Denis Jacquemin: Publication list 1995–2023 (as 11/2023)

A Articles in peer-reviewed journals

1. D. Jacquemin, B. Champagne and J. M. André*
Molecular Orbital Expressions for Approximate Uncoupled Hartree-Fock Second Hyperpolarizabilities. A Pariser-Parr-Pople Assessment for Model Polyacetylene Chains
Chem. Phys. (IF=2.053), **197** (1995) 107–127 doi.

2. D. Jacquemin, B. Champagne*, J. M. André and B. Kirtman
Exploratory Pariser-Parr-Pople Investigation of the Static Longitudinal First Hyperpolarizability of Polymethineimine Chains
Chem. Phys. (IF=2.005), **213** (1996) 217–228 doi.

3. D. Jacquemin*, B. Champagne and J. M. André
Electronic First Hyperpolarizability of Polymethineimine Chains with Donor and Acceptor Groups
Synth. Met. (IF=1.256), **80** (1996) 205–210 doi.

4. B. Champagne*, D. Jacquemin, J. M. André and B. Kirtman
Ab Initio Coupled Hartree-Fock Investigation of the Static First Hyperpolarizability of Model All-Trans Polymethineimine Oligomers of Increasing Size
J. Phys. Chem. A (IF=3.392), **101** (1997) 3158–3165 doi.

5. D. Jacquemin*, B. Champagne and J. M. André
Electron Correlation Effects upon the Static (Hyper)polarizabilities of Push-Pull Conjugated Polyenes and Polyynes
Int. J. Quantum Chem. (IF=1.341), **65** (1997) 679–688 doi.

6. D. Jacquemin*, B. Champagne and B. Kirtman
Ab Initio Static Polarizability and First Hyperpolarizability of Model Polymethineimine Chains. 2. Effects of Conformation and of Substitution by Donor/Acceptor End Groups
J. Chem. Phys. (IF=3.247), **107** (1997) 5076–5087 doi.

7. D. Jacquemin*, J. A. Morales, E. Deumens and Y. Öhrn
Electron Nuclear Dynamics of Proton Collisions with Methane at 30 eV
J. Chem. Phys. (IF=3.247), **107** (1997) 6146–6155 doi.

8. D. Jacquemin*, B. Champagne and J. M. André
Ab Initio Band Structure of Polymethineimine Isomers
J. Chem. Phys. (IF=3.147), **108** (1998) 1023–1030 doi.

9. D. Jacquemin*, B. Champagne and J. M. André
Static First Hyperpolarizability of Small All-Trans Polymethineimine Oligomers. Basis Set and Electron Correlation Effects
J. Mol. Struct. (THEOCHEM) (IF=1.048), **425** (1998) 69–79 doi.

10. D. Jacquemin*, B. Champagne and J. M. André
Møller-Plesset Evaluation of the Static First Hyperpolarizability of Polymethineimine
Chem. Phys. Lett. (IF=2.257), **284** (1998) 24–30 doi.

11. B. Champagne*, E. A. Perpète, T. Legrand, D. Jacquemin and J. M. André
Ab Initio Determination of the Vibrational and Electronic First Hyperpolarizabilities of Reference Compounds for Non-Linear Optical (NLO) Applications: 3-Methyl 4-Nitropyridine 1-Oxide (POM) and N-(4-Nitrophenyl)-(L)-Prolinol (NPP)
J. Chem. Soc. Faraday Trans. (IF=1.757), **94** (1998) 1547–1553 doi.

12. D. Jacquemin*, J. M. André and B. Champagne
Long-Range Effects in Optimizing the Geometry of Stereoregular Polymers. I. Formalism
J. Chem. Phys. (IF=3.289), **111** (1999) 5306–5323 doi.

13. D. Jacquemin*, J. M. André and B. Champagne
Long-Range Effects in Optimizing the Geometry of Stereoregular Polymers. II. Hydrogen Fluoride Chains as a Working Example
J. Chem. Phys. (IF=3.289), **111** (1999) 5324–5330 doi.

14. D. Jacquemin and B. Champagne*
Comment on "Calculation of Ab Initio Hyperpolarizabilities of Polymers" [J. Chem. Phys. 110, 2717 (1999)]
J. Chem. Phys. (IF=3.301), **112** (2000) 1616–1617 doi.

15. D. Jacquemin*, B. Champagne and C. Hättig
Correlated Frequency-Dependent Electronic First Hyperpolarizability of Small Push-Pull Conjugated Chains
Chem. Phys. Lett. (IF=2.364), **319** (2000) 327–334 doi.

16. B. Champagne*, E. A. Perpète, D. Jacquemin, S. van Gisbergen, E. V. Baerends, C. Soubra-Ghaoui, K. A. Robins and B. Kirtman
Assessment of Conventional Density Functional Schemes for Computing the Polarizabilities and First Hyperpolarizabilities of Push-Pull π-Conjugated Systems
J. Phys. Chem. A (IF=2.754), **104** (2000) 4755–4763 doi.

17. M. Spassova, T. Kolev, I. Kanev, D. Jacquemin and B. Champagne*
Structure and Nonlinear Electrical Properties of Squaric Acid Derivatives: A Theoretical Study of the Conformation and Deprotonation Effects
J. Mol. Struct. (THEOCHEM) (IF=0.961), **528** (2000) 151–159 doi.

18. E. A. Perpète*, B. Champagne and D. Jacquemin
Electronic and Vibrational First Hyperpolarizability of Polymethineimine
J. Mol. Struct. (THEOCHEM) (IF=0.961), **529** (2000) 65–71 doi.

19. D. Jacquemin* and B. Champagne
Optimizing the Geometry of Stereoregular Polymers. III. Polyyne and the Problem of Basis Set Linear Dependences
Int. J. Quantum Chem. (IF=1.317), **80** (2000) 863–870 doi.

20. T. D. Poulsen*, K. V. Mikkelsen, J. G. Fripiat, D. Jacquemin and B. Champagne
MP2 Correlation Effects upon the Electronic and Vibrational Properties of Polyyne
J. Chem. Phys. (IF=3.147), **114** (2001) 5917–5922 doi.

21. D. Jacquemin*, B. Champagne, E. A. Perpète, J. M. Luis and B. Kirtman
Second-Order Møller-Plesset Study of Optimum Chain Length for Total (Electronic plus Vibrational) $\beta(-\omega_\sigma;\omega_1,\omega_2)$ of a Prototype Push-Pull Polyene
J. Phys. Chem. A (IF=2.630), **105** (2001) 9748–9755 doi.

22. D. Jacquemin*, D. Beljonne, B. Champagne, V. Geskin, J. L. Brédas and J. M. André
Analysis of the Sign Reversal of the Second-Order Molecular Polarizability of Polymethineimine Chains
J. Chem. Phys. (IF=3.147), **115** (2001) 6766–6774 doi.

23. D. Jacquemin* and B. Champagne
Long-Range Effects in Optimizing the Geometry of Stereoregular Polymers–IV: Explicit Determination of the Helical Angle
Int. J. Quantum Chem. (IF=1.249), **85** (2001) 539–545 doi.

24. D. Jacquemin*, E. A. Perpète and B. Champagne
First Hyperpolarizability of H-(BN)N-H Oligomers: Analysis of Geometry, Asymmetry and Delocalization Effects
Phys. Chem. Chem. Phys. (IF=1.838), **4** (2002) 432–440 doi.

25. D. Jacquemin*, J. G. Fripiat and B. Champagne
Convergence of Exchange Lattice Summations in Direct-Space Polymer Calculations
Int. J. Quantum Chem. (IF=1.514), **89** (2002) 452–463 doi.

26. M. Yang, D. Jacquemin and B. Champagne*
Intramolecular Charge Transfer and First-Order Hyperpolarizability of Planar and Twisted Sesquifulvalenes
Phys. Chem. Chem. Phys. (IF=1.838), **4** (2002) 5566–5571 doi.

27. D. Jacquemin*, B. Champagne, J. M. André, E. Deumens and Y. Öhrn
Integral Algorithm and Density Matrix Integration Scheme for Ab Initio Band Structure Calculations on Polymeric Systems
J. Comput. Chem. (IF=2.931), **23** (2002) 1430–1444 doi.

28. D. Jacquemin*, J. M. André and B. Champagne
Analytic Ab Initio Determination of the Elastic Modulus in Stereoregular Polymers. Analytical Integrals Derivatives, Long-Range Effects, Implementation, and Examples
J. Chem. Phys. (IF=2.950), **118** (2003) 373–388 doi.

29. D. Jacquemin*, J. M. André and B. Champagne
Analytic Ab Initio Determination of the IR Intensities in Stereoregular Polymers
J. Chem. Phys. (IF=2.950), **118** (2003) 3956–3965 doi.

30. D. Jacquemin*, B. Champagne and J. M. André
Copolymerization Effects upon the Second-Order NLO Responses of Polyacetylene/Polymethineimine
Macromolecules (IF=3.621), **36** (2003) 3980–3985 doi.

31. B. Champagne*, D. Jacquemin, F. L. Gu, Y. Aoki, D. M. Bishop and B. Kirtman
Pseudo Linear-Dependence and Long-Range Interaction on the Polarizability and Hyperpolarizabilities of Stereoregular Polymers
Chem. Phys. Lett. (IF=2.438), **373** (2003) 539–549 doi.

32. D. Jacquemin*
Theoretical Study of Dehydrogenation Effects upon the First Hyperpolarizability of Polyphosphinoborane
J. Phys. Chem. A (IF=2.639), **108** (2004) 500–506 doi.

33. D. Jacquemin*, C. Lambert and E. A. Perpète
Structures and Properties of Polyphosphinoborane: an Oligomeric Theoretical Study
Macromolecules (IF=3.898), **37** (2004) 1009–1015 doi.

34. D. Jacquemin*, O. Quinet, B. Champagne and J. M. André
Second-Order Nonlinear Optical Coefficient of Polyphosphazene-Based Materials: a Theoretical Study
J. Chem. Phys. (IF=3.105), **120** (2004) 9401–9409 doi.

35. D. Jacquemin*, E. A. Perpète and J. M. André
Theoretical Study of the Longitudinal First Hyperpolarizability of Polysilaacetylene
J. Chem. Phys. (IF=3.105), **120** (2004) 10317–10327 doi.

36. D. Jacquemin*, J. Preat, M. Charlot, V. Wathelet, J. M. André and E. A. Perpète
Theoretical Investigation of Substituted Anthraquinone Dyes
J. Chem. Phys. (IF=3.105), **121** (2004) 1736–1743 doi.

37. D. Jacquemin*, V. Wathelet and E. A. Perpète
Effects of Chain Substitution on the Structures and Properties of Polyphosphinoborane
Macromolecules (IF=3.898), **37** (2004) 5040–5046 doi.

38. D. Jacquemin*, J. M. André and E. A. Perpète
Geometry, Dipole Moment, Polarizability and First Hyperpolarizability of Polymethineimine: an Assessment of Electron Correlation Contributions
J. Chem. Phys. (IF=3.105), **121** (2004) 4389–4396 doi.

39. D. Jacquemin*
First Hyperpolarizability of Polyaminoborane and Polyiminoborane Oligomers
J. Phys. Chem. A (IF=2.639), **108** (2004) 9260–9266 doi.

40. D. Jacquemin*, E. A. Perpète, V. Wathelet and J. M. André
An Ab Initio Investigation of the Structures and Properties of Polyaminoborane
J. Phys. Chem. A (IF=2.639), **108** (2004) 9616–9624 doi.

41. D. Jacquemin*, X. Assfeld and E. A. Perpète
Solvent Effects on the Geometry and First Hyperpolarizability of Polymethineimine
J. Mol. Struct. (THEOCHEM) (IF=1.007), **710** (2004) 13–17 doi.

42. M. Medved'⋆, J. Noga, D. Jacquemin and E. A. Perpète
Longitudinal NLO Properties of C_2H_2, HCCF, and C_2F_2: Electron Correlation and Vibration Effects
Int. J. Quantum Chem. (IF=1.192), **102** (2005) 209–223 doi.

43. D. Jacquemin⋆
Linear and NonLinear Optics Properties of Polyphosphazene/Polynitrile Copolymers
J. Chem. Theory Comput. (IF=NA, 2006 FI=3.627), **1** (2005) 307–314 doi.

44. D. Jacquemin, E. A. Perpète, I. Ciofini and C. Adamo⋆
Assessment of Recently-Developed Density Functional Approaches for the Evaluation of the Bond Length Alternation in Polyacetylene
Chem. Phys. Lett. (IF=2.438), **405** (2005) 376–381 doi.

45. D. Jacquemin⋆, J. Preat, V. Wathelet, J. M. André and E. A. Perpète
Substitution Effects on the Visible Spectra of 1,4-diNHPh-9,10-Anthraquinone
Chem. Phys. Lett. (IF=2.438), **405** (2005) 429–433 doi.

46. D. Jacquemin⋆, M. Medved' and E. A. Perpète
Linear Phosphorus-Boron Chains: a Model System with Huge Electronic First Hyperpolarizability
Int. J. Quantum Chem. (IF=1.192), **103** (2005) 226–234 doi.

47. D. Y. Zhang, C. Pouchan, D. Jacquemin⋆ and E. A. Perpète
Ab Initio Studies of the Static Electronic First Hyperpolarizability of Polysilanenitrile
Chem. Phys. Lett. (IF=2.438), **408** (2005) 226–231 doi.

48. D. Jacquemin⋆, A. Femenias, H. Chermette⋆, J. M. André⋆ and E. A. Perpète⋆
A Second-Order Møller-Plesset Evaluation of the Bond Length Alternation of Linear Oligomers
J. Phys. Chem. A (IF=2.898), **109** (2005) 5734–5741 doi.

49. D. Jacquemin⋆ and E. A. Perpète
Ab Initio Assessment of the First Hyperpolarizability of Saturated and Unsaturated Polyaminoborane / Polyphosphinoborane Copolymers
J. Phys. Chem. A (IF=2.898), **109** (2005) 6380–6386 doi.

50. D. Jacquemin⋆, J. Preat and E. A. Perpète
A TD-DFT Study of the Absorption Spectra of Fast Dye Salts
Chem. Phys. Lett. (IF=2.438), **410** (2005) 254–259 doi.

51. D. Jacquemin⋆, J. Preat, V. Wathelet and E. A. Perpète
Theoretical Investigation of the Absorption Spectrum of Thioindigo Dyes
J. Mol. Struct. (THEOCHEM) (IF=1.045), **731** (2005) 67–72 doi.

52. J. Preat⋆, D. Jacquemin and E. A. Perpète
Top 25 Hottest Articles
Theoretical Investigation of the UV Spectra of Coumarin Derivatives
Chem. Phys. Lett. (IF=2.438), **415** (2005) 20–24 doi.

53. D. Jacquemin⋆, E. A. Perpète and J. M. André
NLO Response of Polymethineimine and Polymethineimine/Polyacetylene Conformers: Assessment of Electron Correlation Effects
Int. J. Quantum Chem. (IF=1.192), **105** (2005) 553–563 doi.

54. D. Y. Zhang, C. Pouchan, E. A. Perpète and D. Jacquemin⋆
Ab Initio Prediction of Extremely Large First Hyperpolarizability of Polyphosphaacetylene and Polyphosphasilyne
Chem. Phys. Lett. (IF=2.438), **416** (2005) 277–281 doi.

55. L. Briquet, D. P. Vercauteren, E. A. Perpète and D. Jacquemin⋆
Is Solvated Trans-Azobenzene Twisted or Planar?
Chem. Phys. Lett. (IF=2.462), **417** (2006) 190–195 doi.

56. D. Jacquemin⋆, J. Preat, V. Wathelet, M. Fontaine and E. A. Perpète
ISI Web of KNOWLEDGE Transforming Research
HIGHLY CITED
Thioindigo Dyes: Highly Accurate Visible Spectra with TD-DFT
J. Am. Chem. Soc. (IF=7.696), **128** (2006) 2072–2083 doi.

57. D. Jacquemin*, J. Preat, V. Wathelet and E. A. Perpète
Substitution and Chemical Environment Effects on the Absorption Spectrum of Indigo
J. Chem. Phys. (IF=3.166), **124** (2006) 074104 (12 p.) doi.

58. D. Jacquemin* and E. A. Perpète
The $n \rightarrow \pi^*$ Transition in Nitroso Compounds: a TD-DFT Study
Chem. Phys. Lett. (IF=2.462), **420** (2006) 529–533 doi.

59. E. A. Perpète, V. Wathelet, J. Preat, C. Lambert and D. Jacquemin*
Toward a Theoretical Quantitative Estimation of the λ_{max} of Anthraquinones-Based Dyes
J. Chem. Theory Comput. (IF=3.627), **2** (2006) 434–440 doi.

60. D. Jacquemin, E. A. Perpète, G. Scalmani, M. J. Frisch, I. Ciofini and C. Adamo*
Absorption and Emission Spectra in Gas-Phase and Solution Using TD-DFT: Formaldehyde and Benzene as Case Studies
Chem. Phys. Lett. (IF=2.462), **421** (2006) 272–276 doi.

61. V. Wathelet, J. Preat, M. Bouhy, M. Fontaine, E. A. Perpète, J. M. André and D. Jacquemin*
Assessment of PBE0 for Evaluating the Absorption Spectra of Carbonyl Molecules
Int. J. Quantum Chem. (IF=1.182), **106** (2006) 1853–1859 doi.

62. E. A. Perpète, J. Preat, J. M. André and D. Jacquemin*
An Ab Initio Study of the Absorption Spectra of Indirubin, Isoindigo, and Related Compounds
J. Phys. Chem. A (IF=3.047), **110** (2006) 5629–5635 doi.

63. D. Jacquemin*, A. Femenias, H. Chermette, I. Ciofini, C. Adamo, J. M. André, and E. A. Perpète
Assessment of Several Hybrid DFT Functionals for the Evaluation of Bond Length Alternation of Increasingly Long Oligomers
J. Phys. Chem. A (IF=3.047), **110** (2006) 5952–5959 doi.

64. D. Jacquemin*, M. Bouhy and E. A. Perpète
Excitation Spectra of Nitro-Diphenylaniline: Accurate Time-Dependent Density Functional Theory Predictions for Charge-Transfer Dyes
J. Chem. Phys. (IF=3.166), **124** (2006) 204321 (9 p.) doi.

65. J. Preat*, D. Jacquemin, V. Wathelet, J. M. André and E. A. Perpète
TD-DFT Investigation of the UV Spectra of Pyranone Derivatives
J. Phys. Chem. A (IF=3.047), **110** (2006) 8144–8150 doi.

66. D. Jacquemin*, V. Wathelet and E. A. Perpète
Ab Initio Investigation of the $n \rightarrow \pi^*$ Transitions in Thiocarbonyl Dyes
J. Phys. Chem. A (IF=3.047), **110** (2006) 9145–9152 doi.

67. D. Jacquemin* and E. A. Perpète
Ab Initio Calculations of the Colour of Closed-Ring Diarylethenes: TD-DFT Estimates for Molecular Switches
Chem. Phys. Lett. (IF=2.462), **429** (2006) 147–152 doi.

68. D. Jacquemin*, J. Preat, V. Wathelet and E. A. Perpète
Time-Dependent Density Functional Theory Determination of the Absorption Spectra of Naphthoquinones
Chem. Phys. (IF=1.984), **328** (2006) 324–332 doi.

69. J. de Ruyck*, J. Preat, E. A. Perpète, D. Jacquemin and J. Wouters
2,6-Dihydroxyanthraquinone, an Isomer of Well-Known Alizarin Dye
Acta Cryst. E (IF=0.567), **62** (2006) o4503–o4505 doi.

70. D. Jacquemin*, E. A. Perpète, G. Scalmani, M. J. Frisch, X. Assfeld, I. Ciofini and C. Adamo*
TD-DFT Investigation of the Absorption, Fluorescence, and Phosphorescence Spectra of Solvated Coumarins
J. Chem. Phys. (IF=3.166), **125** (2006) 164324 (11 p.) doi.

71. J. Preat*, D. Jacquemin and E. A. Perpète
A TD-DFT Investigation of the Visible Spectra of Fluoro-Anthraquinones
Dyes Pigm. (IF=2.796), **72** (2007) 185–191 doi.

72. J. Preat*, P. F. Loos, X. Assfeld, D. Jacquemin and E. A. Perpète
DFT and TD-DFT Investigation of IR and UV Spectra of Solvated Molecules: Comparison of two SCRF Continuum Models
Int. J. Quantum Chem. (IF=1.368), **107** (2007) 574–585 doi.

73. D. Jacquemin*, E. A. Perpète, H. Chermette, I. Ciofini and C. Adamo
Comparison of Theoretical Approaches for Computing the Bond Length Alternation of Polymethineimine
Chem. Phys. (IF=1.805), **332** (2007) 79–85 doi.

74. D. Jacquemin* and E. A. Perpète
On the Basis Set Convergence of TD-DFT Oscillator Strengths: Dinitrophenylhydrazones as a Case Study
J. Mol. Struct. (THEOCHEM) (IF=1.112), **804** (2007) 31–34 doi.

75. L. Briquet, D. P. Vercauteren, J. M. André, E. A. Perpète and D. Jacquemin*
On the Geometries and UV/Vis Spectra of Substituted Trans-Azobenzenes
Chem. Phys. Lett. (IF=2.207), **435** (2007) 257–262 doi.

76. E. A. Perpète and D. Jacquemin*
An Ab Initio Scheme for Quantitative Predictions of the Visible Spectra of Diarylethenes
J. PhotoChem. PhotoBiol. A: Chem. (IF=1.911), **187** (2007) 40–44 doi.

77. A. D. Laurent, J. M. André, E. A. Perpète and D. Jacquemin*
Hemi-Indigo Photochroms: a Theoretical Investigation
Chem. Phys. Lett. (IF=2.207), **436** (2007) 84–88 doi.

78. D. Jacquemin, X. Assfeld, J. Preat and E. A. Perpète*
Comparison of Theoretical Approaches for Predicting the UV/Vis Spectra of Anthraquinones
Mol. Phys. (IF=1.568), **105** (2007) 325–331 doi.

79. J. Preat*, P. F. Loos, X. Assfeld, D. Jacquemin and E. A. Perpète
Top 25 Hottest Articles
A TD-DFT Investigation of UV Spectra of Pyranoidic Dyes: A NCM vs PCM Comparison
J. Mol. Struct. (THEOCHEM) (IF=1.112), **808** (2007) 85–91 doi.

80. D. Jacquemin*, E. A. Perpète, X. Assfeld, G. Scalmani, M. J. Frisch and C. Adamo*
Top 25 Hottest Articles
The Geometries, Absorption and Fluorescence Wavelengths of Solvated Fluorescent Coumarins: a CIS and TD-DFT Comparative Study
Chem. Phys. Lett. (IF=2.207), **438** (2007) 208–212 doi.

81. D. Jacquemin*, E. A. Perpète, G. Scalmani, M. J. Frisch, R. Kobayashi and C. Adamo*
Top 20
Assessment of the Efficiency of Long-Range Corrected Functionals for Some Properties of Large Compounds
J. Chem. Phys. (IF=3.044), **126** (2007) 144105 (12 p.) doi.

82. D. Jacquemin*, V. Wathelet, J. Preat and E. A. Perpète
Ab Initio Tools for the Accurate Prediction of the Visible Spectra of Anthraquinones
SpectroChim. Acta A (IF=1.511), **67** (2007) 334–341 doi.

83. E. A. Perpète and D. Jacquemin*
Ab Initio Investigation of the Solvent and Electron Correlation Effects on the Geometries and Static First Hyperpolarizabilities of Push-Pull Oligomers
Int. J. Quantum Chem. (IF=1.368), **107** (2007) 2066–2074 doi.

84. D. Jacquemin*, E. A. Perpète, M. Medved', G. Scalmani, M. J. Frisch, R. Kobayashi and C. Adamo*
First Hyperpolarizability of Polymethineimine with Long-Range Corrected Functionals
J. Chem. Phys. (IF=3.044), **126** (2007) 191108 (4 p.) doi.

85. J. Preat*, D. Jacquemin, V. Wathelet, J. M. André and E. A. Perpète
Towards the Understanding of the Chromatic Behaviour of Triphenylmethane Derivatives
Chem. Phys. (IF=1.805), **335** (2007) 177–186 doi.

86. E. A. Perpète, F. Maurel and D. Jacquemin*
TD-DFT Investigation of Diarylethene Dyes with Cyclopentene, Dihydrothiophene, and Dihydropyrrole Bridges
J. Phys. Chem. A. (IF=2.918), **111** (2007) 5528–5535 doi.

87. C. Michaux, J. Wouters, D. Jacquemin* and E. A. Perpète
A Theoretical Investigation of the Hydrated Glycine Cation Energetics and Structures
Chem. Phys. Lett. (IF=2.207), **445** (2007) 57–61 doi.

88. D. Jacquemin*, E. A. Perpète, O. A. Vydrov, G. E. Scuseria and C. Adamo*
Top 20
Assessment of Long-Range Corrected Functionals Performance for $n \rightarrow \pi^*$ Transitions in Organic Dyes
J. Chem. Phys. (IF=3.044), **127** (2007) 094102 (6 p.) doi.

89. M. Medved'*, J. Noga, D. Jacquemin, X. Assfeld and E. A. Perpète
NLO Responses of Small Polymethineimine Oligomers: a CCSD(T) Study
J. Mol. Struct. (THEOCHEM) (IF=1.112), **821** (2007) 160–165 doi.

90. A. D. Laurent, J. M. André, E. A. Perpète and D. Jacquemin*
Photochromic Properties of Dithienylazoles and Other Conjugated Diarylethenes
J. PhotoChem. PhotoBiol. A: Chem. (IF=1.911), **192** (2007) 211–219 doi.

91. D. Jacquemin*, E. A. Perpète, G. Scalmani, M. J. Frisch, I. Ciofini and C. Adamo*
Top 25 Hottest Articles
Fluorescence of 1,8-Naphthalimide: a PCM-TD-DFT Investigation
Chem. Phys. Lett. (IF=2.207), **448** (2007) 3–6 doi.

92. M. Medved'*, M. Stachova, D. Jacquemin, J. M. André and E. A. Perpète
A Generalized Romberg Differentiation Procedure
J. Mol. Struct. (THEOCHEM) (IF=1.112), **847** (2007) 39–46 doi.

93. E. A. Perpète, C. Lambert, V. Wathelet, J. Preat and D. Jacquemin*
Ab Initio Studies of the λ_{max} of Naphthoquinones Dyes
SpectroChim. Acta A (IF=1.511), **68** (2007) 1326–1333 doi.

94. D. Jacquemin* and E. A. Perpète
Evaluation Ab Initio de la Couleur de Diaryléthènes Présentant un Pont Maléimide
Comptes Rendus Chimie (IF=1.305), **10** (2007) 1227–1233 doi.

95. J. de Ruyck, M. Famerée, J. Wouters, E. A. Perpète, J. Preat and D. Jacquemin*
Towards the Understanding of the Absorption Spectra of NAD(P)H/NAD(P)$^+$ as a Common Indicator of Dehydrogenase Enzymatic Activity
Chem. Phys. Lett. (IF=2.207), **450** (2007) 119–122 doi.

96. J. Preat, C. Michaux, A. Lewalle, E. A. Perpète and D. Jacquemin*
Delocalisation in Conjugated Triazene Chromophores: Insights from Theory
Chem. Phys. Lett. (IF=2.169), **451** (2008) 37–42 doi.

97. J. Preat*, D. Jacquemin and E. A. Perpète
Tayloring Standard TDDFT Approaches for Computing UV/Vis Transitions in Thiocarbonyl Chromophores
Int. J. Quantum Chem. (IF=1.317), **108** (2008) 768–773 doi.

98. D. Jacquemin*, E. A. Perpète, G. E. Scuseria, I. Ciofini and C. Adamo*
The Most Highly Cited
TD-DFT Performance for the Visible Absorption Spectra of Organic Dyes: Conventional versus Long-Range Hybrids
J. Chem. Theory Comput. (IF=4.274), **4** (2008) 123–135 doi.

99. D. Jacquemin, E. A. Perpète, I. Ciofini and C. Adamo*
The Most
A Fast and Reliable Theoretical Determination of pK_a^* for Photoacids
J. Phys. Chem. A. (IF=2.871), **112** (2008) 794–796 doi.

100. C. Michaux, J. Wouters, E. A. Perpète and D. Jacquemin*
Microhydration of Protonated Glycine: an Ab Initio Family Tree
J. Phys. Chem. B. (IF=4.189), **112** (2008) 2430–2438 doi.

101. D. Jacquemin*, E. A. Perpète, I. Ciofini and C. Adamo
Revisiting the Relationship Between the Bond Length Alternation and the First Hyperpolarizability with Range-Separated Hybrid Functionals
J. Comput. Chem. (IF=3.390), **29** (2008) 921–925 doi.

102. J. Preat*, D. Jacquemin, D. P. Vercauteren and E. A. Perpète
A Quantitative Prediction of the Electronic Spectra of Thiocarbonyl Chromophore: TD-DFT vs SAC-CI
Theor. Chem. Acc. (IF=2.370), **119** (2008) 463–468 doi.

103. E. A. Perpète, D. Jacquemin, C. Adamo* and G. E. Scuseria
Revisiting the Nonlinear Optical Properties of Polybutatriene and Polydiacetylene with Density Functional Theory
Chem. Phys. Lett. (IF=2.169), **456** (2008) 101–104 doi.

104. P. F. Loos*, J. Preat, A. D. Laurent, C. Michaux, D. Jacquemin, E. A. Perpète and X. Assfeld
Theoretical Investigation of the Geometries and UV/Vis Spectra of Poly(L-Glutamic Acid) Featuring Photochromic Azobenzene Side Chain
J. Chem. Theory Comput. (IF=4.274), **4** (2008) 637–645 doi.

105. D. Jacquemin*, A. Lewalle and E. A. Perpète
Modelling the Acidochromism of Pyridylazulenes
Chem. Phys. Lett. (IF=2.169), **457** (2008) 91–95 doi.

106. D. Jacquemin*, E. A. Perpète, I. Ciofini and C. Adamo*
Top Cited
On the TD-DFT UV/Vis Spectra Accuracy: the Azoalkanes
Theor. Chem. Acc. (IF=2.370), **120** (2008) 405–410 doi.

107. C. Michaux, J. Wouters, E. A. Perpète and D. Jacquemin*
Stepwise Hydration of Protonated Proline
J. Phys. Chem. B (IF=4.189), **112** (2008) 7702–7705 doi.

108. D. Jacquemin*, E. A. Perpète and C. Adamo*
Modelling the UV/Visible Spectrum of Tetrakis(Phenylethynyl)Benzene
J. Mol. Struct. (THEOCHEM) (IF=1.167), **863** (2008) 123–127 doi.

109. C. Michaux, J. Wouters, E. A. Perpète and D. Jacquemin*
Modelling the Microhydration of Protonated Alanine
J. Phys. Chem. B (IF=4.189), **112** (2008) 9896–9902 doi.

110. F. Maurel, A. Perrier, E. A. Perpète and D. Jacquemin*
A Theoretical Study of the Perfluoro-Diarylethenes Electronic Spectra
J. PhotoChem. PhotoBiol. A: Chem. (IF=2.362), **199** (2008) 211–223 doi.

111. J. M. André*, D. Jacquemin, E. A. Perpète, D. P. Vercauteren and V. Wathelet[1]
Assessment of the Accuracy of TD-DFT Absorption Spectra: Substituted Benzenes
Coll. Czech Chem. Commun. (IF=0.784), **73** (2008) 898–908 doi.

112. D. Jacquemin*, E. A. Perpète, G. E. Scuseria, I. Ciofini and C. Adamo*
Top 25 Hottest Articles
Extensive TD-DFT Investigation of the First Electronic Transition in Substituted Azobenzenes
Chem. Phys. Lett. (IF=2.169), **465** (2008) 226–229 doi.

113. J. Casanovas, D. Jacquemin*, E. A. Perpète and C. Alemán*
Fluorescein Isothiocyanante: Molecular Characterization using Theoretical Calculations
Chem. Phys. (IF=1.961), **354** (2008) 155–161 doi.

[1] Alphabetical order list.

114. J. Preat*, D. Jacquemin, J. Burton, D. P. Vercauteren and E. A. Perpète
Quantitative Evaluation of Solvation and Packing Effects on the Visible Absorption Spectra of Anthraquinone Derivatives
Dyes Pigm. (IF=2.855), **81** (2009) 97–102 doi.

115. D. Jacquemin*, E. A. Perpète, A. D. Laurent, X. Assfeld and C. Adamo*
Spectral Properties of Self-Assembled Squaraine-Tetralactam: a Theoretical Assessment
Phys. Chem. Chem. Phys. (IF=4.116), **11** (2009) 1258–1262 doi.

116. D. Jacquemin*, E. A. Perpète, I. Ciofini and C. Adamo*
Most Read Articles
Accurate Simulation of Optical Properties in Dyes
HIGHLY CITED
Acc. Chem. Res. (IF=18.203), **42** (2009) 326–334 doi.

117. C. Michaux, J. Wouters, E. A. Perpète and D. Jacquemin*
Ab Initio Investigation of the Hydration of Deprotonated Amino Acids
J. Am. Soc. Mass. Spectr. (IF=3.391), **20** (2009) 632–638 doi.

118. J. Preat*, A. D. Laurent, C. Michaux, E. A. Perpète and D. Jacquemin
Impact of Tautomers on the Absorption Spectra of Neutral and Anionic Alizarin and Quinizarin Dyes
J. Mol. Struct. (THEOCHEM) (IF=1.216), **901** (2009) 24–30 doi.

119. M. Medved'*, S. Budzak, D. Jacquemin and E. A. Perpète
Enhancement of the Second-Order NLO Responses of Boron-Nitrogen Oligomers by Copolymerization with Polyyne
J. Mol. Struct. (THEOCHEM) (IF=1.216), **901** (2009) 194–201 doi.

120. J. P. Cerón-Carrasco*, A. Requena, C. Michaux, E. A. Perpète and D. Jacquemin
Effects of Hydration on the Proton Transfer Mechanism in the Adenine-Thymine Base Pair
J. Phys. Chem. A (IF=2.899), **113** (2009) 7892–7898 doi.

121. P. Vandurm, C. Cauvin, J. Wouters, E. A. Perpète and D. Jacquemin*
Electronic Transitions of Neutral and Anionic Quinolinone HIV-1 Integrase Inhibitor: Joint Theory/Experiment Investigation
Chem. Phys. Lett. (IF=2.291), **478** (2009) 243–248 doi.

122. D. Jacquemin*, V. Wathelet, E. A. Perpète and C. Adamo*
Most Read Articles
Extensive TD-DFT Benchmark: Singlet-Excited States of Organic Molecules
Most Cited Articles
J. Chem. Theory Comput. (IF=4.804), **5** (2009) 2420–2435 doi.

123. J. Preat*, C. Michaux, D. Jacquemin and E. A. Perpète
Enhanced Efficiency of Organic Dye-Sensitized Solar Cells: Triphenylamine Derivatives
J. Phys. Chem. C (IF=4.224), **113** (2009) 16821–16833 doi.

124. J. P. Cerón-Carrasco*, A. Requena, A. Zuniga, C. Michaux, E. A. Perpète and D. Jacquemin
Intermolecular Proton Transfer in Microhydrated Guanine-Cytosine Base Pairs: a New Mechanism for Spontaneous Mutation in DNA
J. Phys. Chem. A (IF=2.899), **113** (2009) 10549–10556 doi.

125. D. Jacquemin*, A. D. Laurent, E. A. Perpète and J. M. André*
An Ab Initio *Simulation of the UV/Visible Spectra of N-Benzyildeneaniline Dyes*
Int. J. Quantum Chem. (IF=1.315), **109** (2009) 3506–3515 doi.

126. E. A. Perpète and D. Jacquemin*
TD-DFT Benchmark for Indigoïd Dyes
J. Mol. Struct. (THEOCHEM) (IF=1.216), **914** (2009) 100–105 doi.

127. A. Perrier*, F. Maurel, E. A. Perpète, V. Wathelet and D. Jacquemin*
Spectral Properties of Spirooxazine Photochromes: TD-DFT Insights
J. Phys. Chem. A (IF=2.899), **113** (2009) 13004–13012 doi.

128. J. P. Cerón-Carrasco*, A. Requena, E. A. Perpète, C. Michaux and D. Jacquemin
Double Proton Transfer Mechanism in the Adenine-Uracil Base Pair and Spontaneous Mutation in RNA Duplex
Chem. Phys. Lett. (IF=2.291), **484** (2009) 64–68 doi.

129. D. Jacquemin*, E. A. Perpète, F. Maurel and A. Perrier*
Ab Initio Investigation of the Electronic Properties of Coupled Dithienylethenes
J. Phys. Chem. Lett. (IF=6.213), **1** (2010) 434–438 doi.

130. A. D. Laurent*, X. Assfeld, D. Jacquemin, J. M. André and E. A. Perpète
Substitution Effects on the Optical Spectra of Diarylethene Photochroms: Ab Initio Insights
Mol. Simul. (IF=1.215), **36** (2010) 74–78 doi.

131. G. Fayet, D. Jacquemin*, V. Wathelet, E. A. Perpète, P. Rotureau and C. Adamo*
Excited-State Properties from Ground-State DFT Descriptors: a QSPR Approach for Dyes
J. Mol. Graph. Model. (IF=2.033), **28** (2010) 465–471 doi.

132. D. Jacquemin*, C. Michaux, E. A. Perpète, F. Maurel and A. Perrier
Photochromic Molecular Wires: Insights from Theory
Chem. Phys. Lett. (IF=2.280), **488** (2010) 193–197 doi.

133. D. Jacquemin*, E. A. Perpète, I. Ciofini and C. Adamo*
Most Read Articles *Assessment of Functionals for TD-DFT Calculations of Singlet-Triplet Transitions*
HIGHLY CITED J. Chem. Theory Comput. (IF=5.138), **6** (2010) 1532–1537 doi.

134. D. Jacquemin*, E. A. Perpète, F. Maurel and A. Perrier*
Doubly Closing or not ? Theoretical Analysis for Coupled Photochromes
J. Phys. Chem. C (IF=4.520), **114** (2010) 9489–9497 doi.

135. D. Jacquemin*, E. A. Perpète, G. Scalmani, I. Ciofini, C. Peltier and C. Adamo*
Top 25 *Absorption and Emission Spectra of 1,8-Naphthalimide Fluorophores: a PCM-TD-DFT Investigation*
Hottest Articles Chem. Phys. (IF=2.017), **372** (2010) 61–66 doi.

136. D. Jacquemin*, C. Peltier and I. Ciofini*
Visible Spectrum of Naphthazarin Investigated through Time-Dependent Density Functional Theory
Chem. Phys. Lett. (IF=2.280), **493** (2010) 67–71 doi.

137. D. Jacquemin*, E. A. Perpète, F. Maurel and A. Perrier*
Simulation of the Properties of a Photochromic Triad
J. Phys. Chem. Lett. (IF=6.213), **1** (2010) 2104–2108 doi.

138. J. Preat*, D. Jacquemin and E. A. Perpète
Top Ten *Towards New Efficient Dyes Sensitised Solar Cells*
Energy Environ. Sci. (IF=9.446), Perspective Article, **3** (2010) 891–904 doi.

139. D. Jacquemin*, J. Preat, E. A. Perpète and C. Adamo
Absorption Spectra of Recently-Synthesised Organic Dyes: a TD-DFT Study
Int. J. Quantum Chem. (IF=1.302), **110** (2010) 2121–2129 doi.

140. J. Preat*, D. Jacquemin and E. A. Perpète
A UV/Vis Spectra Investigation of pH-Sensitive Dyes using Time-Dependent Density Functional Theory
Int. J. Quantum Chem. (IF=1.302), **110** (2010) 2147–2154 doi.

141. D. Jacquemin*, E. A. Perpète, I. Ciofini, C. Adamo*, R. Valero, Y. Zhao and D. G. Truhlar
Most Read Articles *On the Performances of the M06 Family of Density Functionals for Electronic Excitation Energies*
HIGHLY CITED J. Chem. Theory Comput. (IF=5.138), **6** (2010) 2071–2085 doi.

142. J. Preat*, D. Jacquemin and E. A. Perpète
Design of New Triphenylamine-Sensitized Solar Cells: a Theoretical Approach
Environ. Sci. Technol. (IF=4.825), **44** (2010) 5666–5671 doi.

143. D. Jacquemin*, E. A. Perpète, F. Maurel and A. Perrier
TD-DFT Simulations of the Electronic Properties of Star-Shaped Photochromes
Phys. Chem. Chem. Phys. (IF=3.453), **12** (2010) 7994–8000 doi.

144. C. A. Guido, B. Mennucci, D. Jacquemin and C. Adamo*
Planar vs. *Twisted Intramolecular Charge Transfer Mechanism in Nile Red: New Hints from Theory*
Phys. Chem. Chem. Phys. (IF=3.453), **12** (2010) 8016–8023 doi.

145. D. Jacquemin⋆, C. Peltier and I. Ciofini⋆
On the Absorption Spectra of Recently Synthesized Carbonyl Dyes: TD-DFT Insights
J. Phys. Chem. A (IF=2.732), **114** (2010) 9579–9582 doi.

146. D. Jacquemin⋆, E. A. Perpète, F. Maurel and A. Perrier
Hybrid Dithienylethene-Naphthopyran Multi-Addressable Photochromes: an Ab Initio Analysis
Phys. Chem. Chem. Phys. (IF=3.453), **12** (2010) 13144–13152 doi.

147. A. Tabatchnik-Rebillon, C. Aubé, H. Bakkali, T. Delaunay, G. Thia Manh, V. Blot, C. Thobie-Gautier, E. Renault, A. Planchat, J. Y. Le Questel, B. Kauffmann, Y. Ferrand, I. Huc, K. Urgin, S. Condon, E. Léonel, M. Evain, J. Lebreton, D. Jacquemin, M. Pipelier and D. Dubreuil⋆
Electrochemical Synthesis and Characterisation of Alternated Tripyridyl-Dipyrrole Molecular Strands with Multi Nitrogen-Based Donor/Acceptor Binding Sites
Chem. Eur. J. (IF=5.476), **16** (2010) 11876–11889 doi.

148. J. P. Cerón-Carrasco⋆, A. Requena, E. A. Perpète, C. Michaux and D. Jacquemin
Theoretical Study of the Tautomerism in One-Electron Oxidized Guanine-Cytosine Base Pair
J. Phys. Chem. B. (IF=3.603), **114** (2010) 13439–13445 doi.

149. S. Chabbal⋆, D. Jacquemin, C. Adamo, H. Stoll and T. Leininger
Bond Length Alternation of Conjugated Oligomers: Another Step on the Fifth Rung of Perdew's Ladder of Functional
J. Chem. Phys. (IF=2.920), **133** (2010) 151104 (4 p.) doi.

150. J. Preat⋆, D. Jacquemin, C. Michaux and E. A. Perpète
Top 25 Hottest Articles
Improvement of the Efficiency of Thiophene-Bridged Compounds for Dye-Sensitized Solar Cells
Chem. Phys. (IF=2.017), **376** (2010) 56–68 doi.

151. C. A. Guido⋆, D. Jacquemin, C. Adamo and B. Mennucci
Most Read Articles
On the TD-DFT Accuracy in Determining Single and Double Bonds in Excited-State Structures of Organic Molecules
J. Phys. Chem. A (IF=2.732), **114** (2010) 13402–13410 doi.

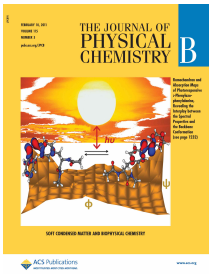
152. D. Jacquemin⋆, E. A. Perpète, F. Maurel and A. Perrier⋆
Top 25 Hottest Articles
Photochromic Properties of a Dithienylethene-Indolinooxazolidine Switch:a Theoretical Investigation
Comput. Theor. Chem. (IF=1.437), **963** (2011) 63–70 doi.

153. E. Dumont⋆, A. D. Laurent, X. Assfeld and D. Jacquemin
Performances of Recently-Proposed Functionals for Describing Disulfide Radical Anions and Similar Systems
Chem. Phys. Lett. (IF=2.337), **501** (2011) 245–251 doi.

154. A. Perrier, F. Maurel, I. Ciofini and D. Jacquemin⋆
A Theoretical Spectroscopy Investigation of Bifunctional Platinum-Bridged Diarylethenes
Chem. Phys. Lett. (IF=2.337), **502** (2011) 77–81 doi.

155. F. Maurel, A. Perrier and D. Jacquemin⋆
An ab initio Simulation of a Dithienylethene/Phenoxynaphthacenequinone Photochromic Hybrid
J. PhotoChem. PhotoBiol. A: Chem. (IF=2.421), **218** (2011) 33–40 doi.

156. D. Jacquemin⋆, E. A. Perpète, I. Ciofini and C. Adamo⋆
Most Cited Articles
HOT PAPERS
Assessment of the ωB97 Family for Excited-state Calculations
Theor. Chem. Acc. (IF=2.162), **128** (2011) 127–136 doi.



157. G. Revilla-Lopez, A. D. Laurent, E. A. Perpète, D. Jacquemin⋆, J. Torres, X. Assfeld⋆ and C. Alemán⋆
Key Building Block of Photoresponsive Biomimetic Systems
J. Phys. Chem. B (IF=3.696), **115** (2011) 1232–1242 doi.

158. D. Jacquemin⋆ and C. Adamo⋆
ISI Web of KNOWLEDGE Transforming Research
HIGHLY CITED
Bond Length Alternation of Conjugated Oligomers: Wave Function and DFT Benchmarks
J. Chem. Theory Comput. (IF=5.215), **7** (2011) 369–376 doi.

159. D. Jacquemin*
New Cyanine Dyes or Not ? Theoretical Insights for Model Chains
J. Phys. Chem. A (IF=2.946), **115** (2011) 2442–2445 doi.

160. D. Jacquemin*, E. A. Perpète, C. Michaux and G. Frison*
Comparison of Microhydration Methods: Protonated Glycine as a Working Example
J. Phys. Chem. B. (IF=3.696), **115** (2011) 3604–3613 doi.

161. Y. Pellegrin, L. Le Pleux, E. Blart, A. Renaud, B. Chavillon, N. Szuwarski, M. Boujtita, L. Cario, S. Jobic, D. Jacquemin* and F. Odobel*
Top 25 Hottest Articles
Ruthenium Polypyridine Complexes as Sensitizers in NiO Based p-type Dye-Sensitized Solar Cells: Effects of the Anchoring Groups
J. PhotoChem. PhotoBiol. A: Chem. (IF=2.421), **219** (2011) 235–242 doi.

162. A. Perrier*, F. Maurel and D. Jacquemin*
Interplay Between Electronic and Steric Effects in Multi-Photochromic Diarylethenes
J. Phys. Chem. C (IF=4.805), **115** (2011) 9193–9203 doi.

163. A. Perrier, F. Maurel and D. Jacquemin*
Nature of the Excited-States in Large Photochromic Dimers: a TD-DFT Examination
Chem. Phys. Lett. (IF=2.337), **509** (2011) 129–133 doi.

164. A. I. Gilson, G. van der Rest, J. Chamot-Rooke, W. Kurlancheek, M. Head-Gordon, D. Jacquemin and G. Frison*
Ground Electronic State of Peptide Cation Radicals: a Delocalized Unpaired Electron ?
J. Phys. Chem. Lett. (IF=6.213), **2** (2011) 1426–1431 doi.

165. D. Jacquemin*, E. Bremond, A. Planchat, I. Ciofini and C. Adamo*
TD-DFT Vibronic Couplings in Anthraquinones: from Basis Set and Functional Benchmarks to Applications for Industrial Dyes
J. Chem. Theory Comput. (IF=5.215), **7** (2011) 1882–1892 doi.

166. A. Perrier*, F. Maurel and D. Jacquemin*
Diarylethene-Dihydroazulene Multimode Photochrome: a Theoretical Spectroscopy Investigation
Phys. Chem. Chem. Phys. (IF=3.573), **13** (2011) 13791–13799 doi.

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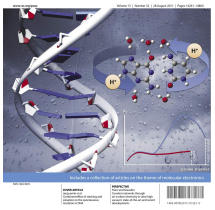

167. J. P. Cerón-Carrasco*, J. Zúñiga, A. Requena, E. A. Perpète, C. Michaux and D. Jacquemin*
Editor's Choice
Combined Effect of Stacking and Solvation on the Spontaneous Mutation in DNA
Phys. Chem. Chem. Phys. (IF=3.573), **13** (2011) 14584–14589 doi.

168. D. Jacquemin*, B. Mennucci* and C. Adamo*
Most downloaded
Excited-State Calculations with TD-DFT: from Benchmarks to Simulations in Complex Environments
Top Ten
Phys. Chem. Chem. Phys. (IF=3.573), Perspective Article, **13** (2011) 16987–16998 doi.

169. J. P. Cerón-Carrasco* and D. Jacquemin*
Influence of Mg^{2+} on the Guanine-Cytosine Tautomeric Equilibrium: Simulations of the Induced Intermolecular Proton Transfer
ChemPhysChem (IF=3.412), **12** (2011) 2615–2623 doi.

170. D. Jacquemin*, J. Preat, E. A. Perpète, D. P. Vercauteren, J. M. André, I. Ciofini and C. Adamo*
Absorption Spectra of Azobenzenes Simulated with Time-Dependent Density Functional Theory
Int. J. Quantum Chem. (IF=1.357), **111** (2011) 4224–4240 doi.

171. J. Y. Le Questel*, J. Graton, J. P. Cerón-Carrasco, D. Jacquemin, A. Planchat and S. Thany*
New Insights on the Molecular Features, Electrophysiological Properties of Imidacloprid, Acetamiprid and Dinotefuran Neonicotinoid Insecticides
Bioorg. Med. Chem. (IF=2.921), **19** (2011) 7623–7634 doi.

172. A. Tilborg, D. Jacquemin, B. Norberg, E. A. Perpète, C. Michaux and J. Wouters*
Structural Study of PIRACETAM *Polymorphs and Cocrystals: Crystallography Redetermination and Quantum Mechanics Calculations*
Acta Cryst. B (IF=2.286), **67** (2011) 499–507 doi.

173. M. Cipolloni, A. Heynderickx, F. Maurel, A. Perrier, D. Jacquemin⋆, O. Siri, F. Ortica and G. Favaro⋆
A Multiswitchable Acidichromic and Photochromic bis*Diarylethene. An Experimental and Theoretical Study*
J. Phys. Chem. C (IF=4.805), **115** (2011) 23096–23106 doi.

174. J. Warnan, L. Favereau, Y. Pellegrin, E. Blart, D. Jacquemin⋆ and F. Odobel⋆
Top 25 Hottest Articles HIGHLY CITED
A Compact Diketopyrrolopyrrole Dye as Efficient Sensitizer in Titanium Dioxide Dye-Sensitized Solar Cells
J. PhotoChem. PhotoBiol. A: Chem. (IF=2.421), **226** (2011) 9–15 doi.

175. J. P. Cerón-Carrasco, A. Ripoche, F. Odobel and D. Jacquemin⋆
Excited-State Nature in Benzodifuranone Dyes: Insights from ab initio *Simulations*
Dyes Pigm. (IF=3.532), **92** (2012) 1144–1152 doi.

176. B. Le Guennic⋆, O. Maury and D. Jacquemin⋆
Aza-Boron-Dipyrromethene Dyes: TD-DFT Benchmarks, Spectral Analysis and Design of Original Near-IR Structures
Phys. Chem. Chem. Phys. (IF=3.829), **14** (2012) 157–164 doi.

177. E. Cauët and D. Jacquemin⋆
A Theoretical Spectroscopy Investigation of Oxosumanenes
Chem. Phys. Lett. (IF=2.145), **519–520** (2012) 49–53 doi.

178. J. Graton, J. Y. Le Questel, B. Legouin, P. Uriac, P. Van de Weghe and D. Jacquemin⋆
Editor's Choice
A DFT-D Evaluation of the Complexation of a Molecular Tweezer with Small Aromatic Molecules
Chem. Phys. Lett. (IF=2.145), **522** (2012) 11–16 doi.

179. F. Maurel, A. Perrier and D. Jacquemin⋆
Ab Initio Modelling of Optical Spectra in pH-Sensitive Diarylethenes
Int. J. Quantum Chem. (IF=1.306), **112** (2012) 1122–1133 doi.

180. D. Jacquemin⋆, E. Bremond, I. Ciofini and C. Adamo⋆
Impact of Vibronic Couplings on Perceived Colors: Two Anthraquinones as Working Example
J. Phys. Chem. Lett. (IF=6.585), **3** (2012) 468–471 doi.

181. J. Hunault, M. Diswall, J. C. Frison, V. Blot, J. Rocher, S. Marionneau-Lambot, T. Oullier, J. Y. Douillard, S. Guillarme, C. Saluzzo, G. Dujardin, D. Jaquemin, J. Graton, J. Y. Le Questel, M. Evain, J. Lebreton, D. Dubreuil, J. Le Pendu and M. Pipelier⋆
3-Fluoro- and 3,3-Difluoro-3,4-dideoxy-KRN7000 Analogues as New Potent Immunostimulator Agents: Total Synthesis and Biological Evaluation in Human iNKT Cells and Mice
J. Med. Chem. (IF=5.614), **55** (2012) 1227–1241 doi.

182. J. P. Cerón-Carrasco⋆, A. Requena and D. Jacquemin⋆
Impact of DFT Functionals on the Predicted Magnesium-DNA Interaction: an ONIOM Study
Theor. Chem. Acc. (IF=2.233), **131** (2012) 1188 (9 p.) doi.

183. D. Jacquemin⋆
Spectroscopic Properties of Mono- and Bis-Azopyrroles
Int. J. Quantum Chem. (IF=1.306), **112** (2012) 2043–2050 doi.

184. D. Jacquemin⋆ and C. Adamo⋆
Basis Set and Functional Effects on Excited-State Properties: Three Bicyclic Chromogens as Working Examples
Int. J. Quantum Chem. (IF=1.306), **112** (2012) 2135–2141 doi.

185. C. Dupont, E. Dumont⋆ and D. Jacquemin⋆
Superior Performance of Range-Separated Hybrid Functionals for Describing $\sigma^\star \leftarrow \sigma$ UV-Vis Signatures of Three-Electron Two-Center Anions
J. Phys. Chem. A (IF=2.771), **116** (2012) 3237–3246 doi.

186. D. Jacquemin⋆, T. Le Bahers, C. Adamo and I. Ciofini⋆
Most Read Articles
What is the "Best" Atomic Charge Model to Describe Through-Space Charge-Transfer Excitations ?
Phys. Chem. Chem. Phys. (IF=3.829), **14** (2012) 5383–5388 doi.

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Most Read Articles *Verdict: Time-Dependent Density Functional Theory "Not Guilty" of Large Errors for Cyanines*
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Most Read Articles *A Qualitative Failure of B3LYP for Textbook Organic Reactions*
Phys. Chem. Chem. Phys. (IF=3.829), **14** (2012) 7170–7175 doi.

189. A. Perrier*, S. Tesson, D. Jacquemin and F. Maurel
On the Photochromic Properties of Dithienylethenes Grafted on Gold Clusters
Comput. Theor. Chem. (IF=1.371), **990** (2012) 167–176 doi.

190. I. Ciofini, T. Le Bahers, C. Adamo, F. Odobel and D. Jacquemin*
Trough-Space Charge-Transfer in Rod-Like Molecules: Lessons from Theory
J. Phys. Chem. C (IF=4.814), **116** (2012) 11946–11955 doi; errata: **116** (2012) 14736–14736 doi.

191. D. E. López-Pérez, G. Revilla-López, D. Jacquemin, D. Zanuy, B. Palys, S. Sek* and C. Alemán*
Intermolecular Interactions in Electron Transfer through Stretched Helical Peptides
Phys. Chem. Chem. Phys. (IF=3.829), **14** (2012) 10332–10344 doi.

192. D. Bousquet, C. Peltier, C. Masselin, D. Jacquemin, C. Adamo and I. Ciofini*
A DFT Study of Magnetic Interactions in Photoswitchable Systems: Diarylethene Derivatives
Chem. Phys. Lett. (IF=2.145), **542** (2012) 13–18 doi.

193. D. Jacquemin*, A. Planchat, C. Adamo* and B. Mennucci*
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HIGHLY CITED J. Chem. Theory Comput. (IF=5.389), **8** (2012) 2359–2372 doi.

194. J. Warnan, L. Favereau, F. Meslin, M. Severac, E. Blart, Y. Pellegrin, D. Jacquemin* and F. Odobel*
Diketopyrrolopyrrole-Porphyrin Conjugates as Broadly Absorbing Sensitizers for Dye-Sensitized Solar Cells
ChemSusChem (IF=7.475), **5** (2012) 1568–1577 doi.

195. P. O. Hubin, D. Jacquemin, L. Leherte, J. M. André, A. C. T. van Duin and D. P. Vercauteren*
Ab Initio Quantum Mechanical and ReaxFF-based Study of the Intramolecular Iminium-Enamine Conversion in a Proline-Catalyzed Reaction
Theor. Chem. Acc. (IF=2.233), **131** (2012) 1261 (11p) doi.

196. A. Perrier, F. Maurel and D. Jacquemin*
Single Molecule MultiPhotochromism with Diarylethenes
Acc. Chem. Res. (IF=20.833), **45** (2012) 1173–1182 doi.

197. J. P. Cerón-Carrasco, D. Jacquemin* and E. Cauët
Cisplatin Cytotoxicity: a Theoretical Study of Induced Mutations
Phys. Chem. Chem. Phys. (IF=3.829), **14** (2012) 12457–12464 doi.

198. S. Chibani, B. Le Guennic,* A. Charaf-Eddin, O. Maury, C. Andraud and D. Jacquemin*
On the Computation of Adiabatic Energies in Aza-Boron-Dipyrromethene Dyes
J. Chem. Theory Comput. (IF=5.389), **8** (2012) 3303–3313 doi.

199. H. Nitadori, L. Ordronneau, J. Boixel, D. Jacquemin*, A. Boucekkine, A. Singh, M. Akita, I. Ledoux, V. Guerchais and H. Le Bozec*
Photoswitching of the Second-order Nonlinearity of a Tetrahedral Octupolar Multi DTE-based Copper(I) Complex
Chem. Comm. (IF=6.378), **48** (2012) 10395–10397 doi.

200. J. Graton,* B. Legouin, F. Besseau, P. Uriac, J. Y. Le Questel,
P. van de Weghe and D. Jacquemin*
Molecular Tweezers in Host-Guest Complexes: A Computational Study through a DFT-D Approach
J. Phys. Chem. C (IF=4.814), **116** (2012) 23067–23074 doi.

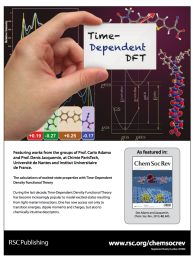
201. E. Göransson, J. Boixel, J. Fortage, D. Jacquemin*, H. C. Becker, E. Blart, L. Hammarström* and F. Odobel*
Most Read Articles *Long-Range Electron Transfer in Zinc-Phthalocyanine-oligo(phenylene-ethynylene)-based Donor-Bridge-Acceptor Dyads*
Inorg. Chem. (IF=4.593), **51** (2012) 11500–11512 doi.

202. J. P. Cerón-Carrasco and D. Jacquemin*
Interplay Between Hydroxyl Radical Attack and H-bond Stability in Guanine-Cytosine
RSC Adv. (IF=2.562), **2** (2012) 11867–11875 doi.

203. F. B. Anne, N. Galland and D. Jacquemin*
Computing Redox Potentials for Dyes Used in p-type Dye-Sensitized Solar Cells
Int. J. Quantum Chem. (IF=1.306), **112** (2012) 3763–3768 doi.

204. J. P. Cerón-Carrasco, M. Fanuel, A. Charaf-Eddin and D. Jacquemin*
Interplay Between Solvent Models and Predicted Optical Spectra: a TD-DFT Study of 7-OH-Coumarin
Chem. Phys. Lett. (IF=1.991), **556** (2013) 122–126 doi.

205. U. Bussy, I. Tea, V. Ferchaud-Roucher, M. Krempf, V. Silvestre, N. Galland, D. Jacquemin, M. Andresen-Bergström, U. Jurva and M. Boujtita*
Mass Voltammetry Technique in the Presence of Isotopic ^{18}O Labelled Water For the Prediction of Oxidative Metabolism
Anal. Chim. Acta (IF=4.517), **762** (2013) 39–46 doi.



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206. C. Adamo and D. Jacquemin*
The Calculations of Excited-State Properties with Time-Dependent Density Functional Theory
HIGHLY CITED Chem. Soc. Rev. (IF=30.425), *invited tutorial review*, **42** (2013) 845–856 doi.

207. J. P. Cerón-Carrasco* and D. Jacquemin
Electric-Field Induced Mutation on DNA: a Theoretical Investigation of the GC Base Pair
Phys. Chem. Chem. Phys. (IF=4.198), **15** (2013) 4548–4553 doi.
Part of the *great articles recently published in the fields of biophysics and biophysical chemistry.*

208. M. Medved* and D. Jacquemin
Tuning the NLO Properties of Polymethineimine Chains by Chemical Substitution
Chem. Phys. (IF=2.028), **415** (2013) 196–206 doi.

209. S. Chibani, B. Le Guennic*, A. Charaf-Eddin, A. D. Laurent and D. Jacquemin*
Revisiting the Optical Signatures of BODIPY with Ab Initio Tools
Chem. Sci. (IF=8.601), **4** (2013) 1950–1963 doi.

210. S. Aloïse*, M. Silwa, G. Buntinx, S. Delbaere, A. Perrier, F. Maurel, D. Jacquemin and M. Takeshita
Do Inverse Dithienylethene Behave as Normal One ? A Joint Spectroscopic and Theoretical Investigation
Phys. Chem. Chem. Phys. (IF=4.198), **15** (2013) 6226–6234 doi.

211. J. P. Cerón-Carrasco*, D. Jacquemin, J. Graton, S. Thany and J. Y. Le Questel*
New Insights on the Molecular Recognition of Imidacloprid with Aplysia Californica AChBP : a Computational Study
J. Phys. Chem. B (IF=3.377), **117** (2013) 3944–3953 doi.

212. A. Perrier, F. Maurel, W. R. Browne and D. Jacquemin*
Most Read Articles *Full Ring Closing in a Diarylethene Hexamer: Insights from Theory*
Chem. Comm. (IF=6.718), *invited communication*, **49** (2013) 4247–4249 doi.

213. J. Warnan, V. M. Guerin, F. B. Anne, Y. Pellegrin, E. Blart, D. Jacquemin*, T. Pauporté* and F. Odobel*
Ruthenium Sensitizer Functionalized by Acetylacetone Anchoring Groups for Dye-Sensitized Solar Cells
J. Phys. Chem. C (IF=4.835), **117** (2013) 8652–8660 doi.

214. B. Le Guennic⋆, S. Chibani, A. Charaf-Eddin, J. Massue, R. Ziessel, G. Ulrich⋆ and D. Jacquemin⋆
The NBO Pattern in Luminescent Chromophores: Unravelling Excited-State Features with TD-DFT
Phys. Chem. Chem. Phys. (IF=4.189), **15** (2013) 7534–7540 doi.

215. L. Ordronneau, V. Aubert, V. Guerchais, A. Boucekkine, H. Le Bozec⋆, A. Singh, I. Ledoux, and D. Jacquemin⋆
The First Hexa-Dithienylethene Tris(Bipyridine)Metal complexes as Quadratic NLO Photoswitches: Combined Experimental and DFT Studies
Chem. Eur. J. (IF=5.696), **19** (2013) 5845–5849 doi.

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PHYS.ORG *A Water Soluble Probe with Polarity-Induced near Infra-Red Fluorescence and its use in Two-Photon Cerebral Vasculature Imaging*
Chem. Sci. (IF=8.610), **4** (2013) 2833–2843 doi.

218. Z. Chen, M. Giorgi, D. Jacquemin⋆, M. Elhabiri and O. Siri⋆
Hot Papers *Azacalixphyrin: the Hidden Porphyrin Cousin Brought to Light*
Angew. Chem. Int. Ed. (IF=11.336), **52** (2013) 6250–6254 doi.
Selected in Synfacts **9** (2013) 0838 doi.

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Most Read Articles *Choosing a Functional for Computing Absorption and Fluorescence Band Shapes with TD-DFT*
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Diketopyrrolopyrrole-Zinc Porphyrin, a Tuned Panchromatic Association for Dye-Sensitized Solar Cells
J. Mater. Chem. A (IF=7.443), **1** (2013) 7572–7575 doi.

221. A. Perrier⋆, S. Aloïse, M. Olivucci⋆ and D. Jacquemin⋆
Inverse versus Normal Dithienylethenes: A Theoretical investigation of the Photocyclization Reaction
J. Phys. Chem. Lett. (IF=6.687), **4** (2013) 2190–2196 doi.

222. U. Bussy, M. Delaforge, C. El-Bekkali, V. Ferchaud-Roucher, M. Krempf, I. Tea, N. Galland, D. Jacquemin and M. Boujtita⋆
Acebutolol and Alprenolol Metabolism Predictions: Comparative Study of Electrochemical and Cytochrome P450-Catalyzed Reactions Using Liquid Chromatography Coupled to High-Resolution Mass Spectrometry
Anal. Bioanal. Chem. (IF=3.578), **405** (2013) 6077–6085 doi.

223. Y. Houari, D. Jacquemin and A. D. Laurent⋆
Methodological Keys for Accurate pK_a^* Simulations
Phys. Chem. Chem. Phys. (IF=4.189), **15** (2013) 11875–11882 doi.

224. S. Chibani, A. Charaf-Eddin, B. Le Guennic⋆ and D. Jacquemin⋆
Boranil and Related NBO Dyes: Insights From Theory
J. Chem. Theory Comput. (IF=5.310), **9** (2013) 3127–3135 doi.

225. A. Faucon, R. Lenk, J. Hémez, E. Gautron, D. Jacquemin, J.Y. Le Questel, J. Graton, A. Brosseau and E. Ishow⋆
Fluorescent Carboxylic and Phosphonic Acids: Comparative Photophysics from Solution to Organic Nanoparticles
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226. A. D. Laurent and D. Jacquemin*
Most Accessed *TD-DFT Benchmarks: a Review*
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227. J. P. Cerón-Carrasco* and D. Jacquemin*
Electric Field Induced DNA Damage: an Open Door for Selective Mutations
Chem. Comm. (IF=6.718), **49** (2013) 7578–7580 doi.

228. A. Planchat and D. Jacquemin*
Optical Signatures of Boron Adducts of Oxasmaragdyrin: Insights from Theory
Mol. Phys. (IF=1.642), **111** (2013) 1303–1307 doi.

229. F. B. Anne, F. D. Purpan and D. Jacquemin*
Charge-Transfer in QuasiLinear Push-Pull Polyene Chains
Chem. Phys. Lett. (IF=1.991), **581** (2013) 52–56 doi.

230. K. Yuan, J. Boixel, H. Le Bozec, A. Boucekkine, H. Doucet*, V. Guerchais* and D. Jacquemin*
Perfluorocyclohexene Bridges in Inverse Diarylethenes: Synthesis through Pd-Catalysed C-H bond Activation, Experimental and Theoretical Studies on Their Photoreactivity
Chem. Comm. (IF=6.718), **49** (2013) 7896–7898 doi.

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Spectral Signatures of Thieno[3,4-b]pyrazines: Theoretical Interpretations and Design of Improved Structures
Dyes Pigm. (IF=3.468), **99** (2013) 972–978 doi.

233. Y. Houari, D. Jacquemin and A. D. Laurent*
TD-DFT Study of the pK_a^* of Coumarins
Chem. Phys. Lett. (IF=1.991), **583** (2013) 218–221 doi.

234. R. Paulino Neto, D. Jacquemin, C. Adamo and I. Ciofini*
Probing the Performances of HISS Functionals for the Description of Excited States of Molecular Systems
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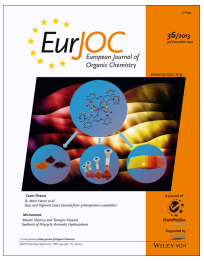
236. G. Fabregat, G. Ballano, J. Casnovas, A. D. Laurent, E. Armelin, L. J. del Valle, C. Cativiela*, D. Jacquemin* and C. Aleman*
Design of Hybrid Conjugates Based on Chemical Similarity
RSC Adv. (IF=3.708), **3** (2013) 21069–21083 doi.

237. Y. Houari, A. D. Laurent and D. Jacquemin*
Spectral Signatures of Perylene Diimide Derivatives: Insights from Theory
J. Phys. Chem. C (IF=4.835), **117** (2013) 21682–21691 doi.

238. O. Selaimia-Ferdjani, A. Kar, S. P. Chavan, M. Horeau, G. Viault, J. Pouessel, X. Guillory, V. Blot, A. Tessier, C. Bidjou-Haiour, A. Planchat, D. Jacquemin, D. Dubreuil and M. Pipelier*
Stereoselective Synthesis of a Bicyclic Norsesquiterpene Backbone. A Possible Route to Nardosinane Derivatives
Eur. J. Org. Chem. (IF=3.154), (2013) 7083–7094 doi.

239. K. Beydoun, M. Zaarour, J. A. Gareth Williams, T. Roisnel, V. Dorcet, A. Planchat, A. Boucekkine, D. Jacquemin*, H. Doucet* and V. Guerchais*
Palladium-Catalysed Direct Arylation of Luminescent Bis-Cyclometallated Iridium(III) Complex Incorporating $\hat{C}N$- *or* $O\hat{O}$-*Coordinating Thiophene-Based Ligands: an Efficient Method for Color tuning*
Inorg. Chem. (IF=4.794), **52** (2013) 12416–12428 doi.

240. B. Yassine, X. Leray, C. Falaise, S. Quinchard, J. P. Ceron-Carrasco, D. Jacquemin, J. Graton, J. Y. Le Questel, S. H. Thany*
Pretreatment of the Cockroach Cercal Afferent/Giant Interneuron Synapses with Nicotinoids and Neonicotinoids Differently Affects Acetylcholine and Nicotine-Induced Ganglionic Depolarizations
Invertebr. Neurosci. (IF=1.192), **13** (2013) 91–97 doi.



241. S. Aiken, C. D. Gabbutt, L. J. Gillie, J. D. Heywood, D. Jacquemin, C. R. Rice and B. M. Heron*
The Remarkable Hyperchromicity of Ketohydrazone Dyes and Pigment Lakes Derived from 4-Morpholino-2-Naphthol
Eur. J. Org. Chem. (IF=3.154), (2013) 8097–8107 doi.

242. J. P. Ceron-Carrasco*, D. Jacquemin and E. Dumont*
Impact of DNA Environment on the Intrastrand Cross-Link Lesions: Hydrogen Atom Release as the Last Step of Formation of G[8-5m]T
J. Phys. Chem. B (IF=3.377), **117** (2013) 16397–16404 doi.

243. Y. Houari, A. Charaf-Eddin, A. D. Laurent, J. Massue, R. Ziessel, G. Ulrich and D. Jacquemin*
Modeling Optical Signatures and Excited-State Reactivities of Substituted HydroxyphenylBenzOxazoles (HBO) ESIPT Dyes
Phys. Chem. Chem. Phys. (IF=4.493), **16** (2014) 1319–1321 doi.

244. A. Charaf-Eddin, B. Le Guennic, and D. Jacquemin*
Optical Signatures of Borico Dyes: a TD-DFT Analysis
Theor. Chem. Acc. (IF=2.233), **133** (2014) 1456 (9p) doi.

245. S. Chibani, A. Charaf-Eddin, B. Mennucci*, B. Le Guennic* and D. Jacquemin*
Most Read Articles
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Strategies for Designing Diarylethenes as Efficient Nonlinear Optical Switches
J. Phys. Chem. C (IF=4.772), **118** (2014) 4334–4345 doi.

247. J. Warnan, Y. Pellegrin, E. Blart, L. Zhang, A. Brown, L. Hammarström*, D. Jacquemin* and F. Odobel*
Acetylacetone Anchoring Group for NiO-Based Dye-Sensitized Solar Cell
Dyes Pigm. (IF=3.966), **105** (2014) 174–179 doi.

248. X. Cui, A. Charaf-Eddin, J. Wang, B. Le Guennic, J. Zhao* and D. Jacquemin*
Perylene-Derived Triplet Acceptors with Optimized Excited State Energy Levels for Triplet-triplet Annihilation Upconversion
J. Org. Chem. (IF=4.721), **79** (2014) 2038–2048 doi.

249. P. Boulanger, D. Jacquemin*, I. Duchemin and X. Blase*
Fast and Accurate Electronic Excitations in Cyanines with the Many-Body Bethe-Salpeter Approach
J. Chem. Theory Comput. (IF=5.498), **10** (2014) 1212–1218 doi.

250. P. O. Hubin*, D. Jacquemin, L. Leherte and D. P. Vercauteren
Quantum Mechanical Investigations on the Role of Neutral and Negatively Charged Enamine Intermediates in Organocatalyzed Reactions
Chem. Phys. (IF=1.652), **434** (2014) 30–36 doi

251. A. D. Laurent*, Y. Houari, P. H. P. R. Carvalho, B. A. D. Neto and D. Jacquemin*
ESIPT or not ESIPT ? Revisiting Recent Results on 2,1,3-Benzothiadiazole under the TD-DFT Light
RSC Adv. (IF=3.840), **4** (2014) 14189–14192 doi.

252. N. Oger, F. Le Callonnec, D. Jacquemin*, E. Fouquet, E. Le Grognec and F.X. Felpin*
Heck-type Arylation of Olefins Through a Double Catalytic Activation of Anilines: Improved Procedures and Rationalization
Adv. Synth. Catal. (IF=5.663), **356** (2014) 1065–1071 doi.

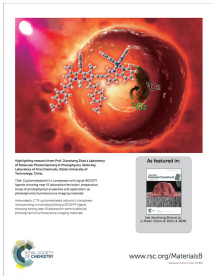
253. J. P. Ceron-Carrasco, H. M. Roy, J. Cerezo, D. Jacquemin and A. D. Laurent*
Theoretical Insights on the Antioxidant Activity of Edaravone Free Radical Scavengers
Chem. Phys. Lett. (IF=1.897), **599** (2014) 73–79 doi.

254. D. Jacquemin*, B. Moore II, A. Planchat, C. Adamo and J. Autschbach*
Performance of an Optimally-Tuned Range-Separated Hybrid Functional for 0-0 Electronic Excitation Energies
J. Chem. Theory Comput. (IF=5.498), **10** (2014) 1677–1685 doi.

255. J. P. Ceron-Carrasco*, J. Cerezo and D. Jacquemin*
How DNA is Damaged by External Electric Fields: Selective Mutation vs. *Random Degradation*
Phys. Chem. Chem. Phys. (IF=4.493), **16** (2014) 8243–8246 doi.

256. J. Boixel, V. Guerchais*, H. Le Bozec, D. Jacquemin*, A. Amar*, A. Boucekkine*, A. Colombo, C. Dragonetti, D. Marinotto, D. Roberto*, S. Righetto and R. De Angelis
Second-Order NLO switches from Molecules to Polymer Films Based on Photochromic Cyclometalated platinum(II) Complexes
J. Am. Chem. Soc. (IF=12.113), **136** (2014) 5367–5375 doi.

257. C. Katan*, P. Savel, B. M. Wong, T. Roisnel, V. Dorcet, J. L. Fillaut and D. Jacquemin*
Absorption and Fluorescence Signatures of 1,2,3-Triazole Based Regioisomers : Challenging Compounds for TD-DFT
Phys. Chem. Chem. Phys. (IF=4.493), **16** (2014) 9064–9073 doi.



258. P. Majumdar, X. Yuan, S. Li, B. Le Guennic, J. Ma, C. Zhang, D. Jacquemin and J. Zhao*
Cyclometalated Ir(III) Complex with Styryl-Bodipy Ligands Showing Near IR Absorption/Emission: Preparation, Study of Photophysical Properties and Application as Photodynamic/Luminescence Imaging Materials
J. Mater. Chem. B (IF=4.726), **2** (2014) 2838–2854 doi.

259. A. Honraedt, M. A. Raux, E. Le Grognec, D. Jacquemin and F. X. Felpin*
Most Read Articles
Copper-Catalyzed Free-Radical C-H Arylation of Pyrroles
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260. J. P. Ceron-Carrasco, D. Jacquemin, C. Laurence*, A. Planchat, C. Reichardt and K. Sraïdi[2]
Determination of a Solvent Hydrogen-bond Acidity Scale by Means of the Solvatochromism of Pyridinium-N-Phenolate Betaine Dye 30 and PCM-TD-DFT Calculations
J. Phys. Chem. B (IF=3.302), **118** (2014) 4605–4614 doi.

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Most Accessed
Solvent Polarity Scales: Determination of New $E_T(30)$ Values for 84 Organic Solvents
J. Phys. Org. Chem. (IF=1.380), **27** (2014) 512–518 doi.

263. A. D'Aléo*, H. Vasile, G. Michel, B. Le Guennic*, D. Jacquemin and F. Fages
NIR Emission in Borondifluoride Complexes of 2'-Hydroxychalcone Derivatives Containing an Acetonaphthone Ring
J. Phys. Chem. C (IF=4.772), **118** (2014) 11906–11918 doi.

264. S. Pascal, A. Haefele, C. Monnereau, A. Charaf-Eddin, D. Jacquemin, B. Le Guennic*, C. Andraud* and O. Maury*
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J. Phys. Chem. A (IF=2.693), **118** (2014) 4038–4047 doi.

[2]Alphabetical author list.
[3]Alphabetical author list.

265. M. Gennari, F. Légalité, L. Zhang, Y. Pellegrin, E. Blart, J. Fortage, A. M. Brown, A. Deronzier, M. C. Collomb⋆, M. Boujtita⋆, D. Jacquemin⋆, L. Hammarström⋆ and F. Odobel⋆
Long-Lived Charge Separated State in NiO based p-type Dye Sensitized Solar Cells with Simple Cyclometalated Iridium Complexes
J. Phys. Chem. Lett. (IF=7.458), **5** (2014) 2254–2258 doi.

266. S. Aiken, K. Booth, C. D. Gabbutt, M. Heron⋆, C. R. Rice, A. Charaf-Eddin and D. Jacquemin
The First Structural and Spectroscopic Characterisation of a Ring-Opened Form of a 2H-Naphtho[1,2-b]pyran; a Novel Photomerocyanine
Chem. Comm. (IF=6.834), **50** (2014) 7900–7903 doi.

267. A. D. Laurent, C. Adamo⋆ and D. Jacquemin⋆
Most Read Articles *Dye Chemistry with Time-Dependent Density Functional Theory*
Phys. Chem. Chem. Phys. (IF=4.493), **16** (2014) 14334–14356 doi.

268. S. Gauthier⋆, B. Caro, F. Robin-Le Guen, N. Bhuvanesh, J. A. Gladysz, L. Wojcik, N. Le Poul, A. Planchat, Y. Pellegrin, E. Blart, D. Jacquemin⋆ and F. Odobel⋆
Synthesis, Photovoltaic Performances and ab initio Modeling of Push-Pull Diacetylide Platinum Complexes in TiO_2 based Dye-Sensitized Solar Cells
Dalton Tans. (IF=4.197), *invited paper*, **43** (2014) 11233–11242 doi.

269. A. Steffen⋆, K. Costuas⋆, A. Boucekkine, M. H.Thibault, A. Beeby, A. S. Batsanov, A. Charaf-Eddin, D. Jacquemin, J.F. Halet and T. B. Marder⋆
Fluorescence in Rhoda- and Iridacyclopentadienes Neglecting the Heavy Atom's Spin-Orbit Coupling: The Ligand Wins
Inorg. Chem. (IF=4.762), **53** (2014) 7055–7069 doi.

270. J. Massue⋆, K. Benelhadj, S. Chibani, B. Le Guennic, D. Jacquemin⋆, P. Retailleau, G. Ulrich⋆ and R. Ziessel⋆
Fluorescent 2-(2'-Hydroxybenzofurane)benzoxazole (HBBO) Borate Complexes: Synthesis, Optical Properties and Theoretical Simulations
Tetrahedron Lett. (IF=2.379), **55** (2014) 4136–4140 doi.

271. C. Laurence⋆, J. Legros, P. Nicolet, D. Vuluga, A. Chantzis and D. Jacquemin
The Solvatomagnetic Comparison Method: a Proper Quantification of Solvent Hydrogen-Bond Basicity
J. Phys. Chem. B (IF=3.302), **118** (2014) 7594–7608 doi.

272. S. Chibani, D. Jacquemin⋆ and A. D. Laurent
Top 25 *Modelling Solvent Effects on the Absorption and Emission Spectra of Constrained Cyanines with both Implicit and Explicit QM/EFP Models*
Hottest Articles Comput. Theor. Chem. (IF=1.545), *invited article*, **1040–1041** (2014) 321–327 doi.

273. D. Jacquemin⋆, S. Chibani, B. Le Guennic and B. Mennucci⋆
Most Read Articles *Solvent Effects on Cyanine Derivatives: a PCM Investigation*
J. Phys. Chem. A (IF=2.693), **118** (2014) 5343–5348 doi.

274. S. Budzak, M. Medved⋆, B. Mennucci and D. Jacquemin⋆
Unveiling Solvents Effect on Excited-State Polarizabilities with the Corrected Linear-Response Model
J. Phys. Chem. A (IF=2.693), **118** (2014) 5652-5656 doi.

275. K. Yuan, J. Boixel, A. Chantzis, D. Jacquemin,⋆ V. Guerchais⋆ and H. Doucet⋆
Benzothiophene or Benzofuran Bridges in DiArylEthenes: Two Steps Synthesis through Sequential Pd-Catalysed C-H bond Activations and Joint Theoretical-Experimental Studies on Their Photoreactivity
Chem. Eur. J. (IF=5.731), **20** (2014) 10073–10083 doi.

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277. V. Riffet, D. Jacquemin, E. Cauët and G. Frison*
Benchmarking DFT and TD-DFT Functionals for the Ground ans Excited States of Hydrogen-Rich Peptide Radicals
J. Chem. Theory Comput. (IF=5.498), **10** (2014) 3308–3318 doi.

278. A. Amar, H. Meghezzi, J. Boixel, H. Le Bozec, V. Guerchais*, D. Jacquemin and A. Boucekkine*
Aggregation Effect on the Luminescence Properties of Phenyl Bipyridine Pt(II) Acetylide Complexes. A Theoretical Prediction with Experimental Evidence.
J. Phys. Chem. A (IF=2.693), **118** (2014) 6278–6286 doi.

279. D. Jacquemin, J. Zuniga, A. Requena and J. P. Ceron-Carrasco*
Assessing the Importance of Proton Transfer Reactions in DNA
Acc. Chem. Res. (IF=22.323), **47** (2014) 2467–2474 doi.

280. A. Chantzis, J. Cerezo, A. Perrier, F. Santoro* and D. Jacquemin*
Optical Properties of Diarylethenes with TD-DFT: 0-0 Energies, Fluorescence, Stokes Shifts and Vibronic Shapes
J. Chem. Theory Comput. (IF=5.498), **10** (2014) 3944–3957 doi.

281. D. Bousquet, R. Fukuda, D. Jacquemin, I. Ciofini, C. Adamo* and M. Ehara*
Benchmark Study on the Triplet Excited-State Geometries and Phosphorescence Energies of Heterocyclic Compounds: Comparison between TD-PBE0 and SAC-CI
J. Chem. Theory Comput. (IF=5.498), **10** (2014) 3969–3979 doi.

282. K. Benelhadj, W. Muzuzu, J. Massue*, P. Retailleau, A. Charaf-Eddin, A. D. Laurent, D. Jacquemin,* G. Ulrich* and R. Ziessel*
White Solid-State Emitters by Tuning the Excited State Intramolecular Proton Transfer (ESIPT) Fluorescence Emission in 2-(2'-Hydroxybenzofuran)benzoxazole (HBBO) Dyes
Chem. Eur. J. (IF=5.731), **20** (2014) 12843–12857 doi.

283. G. Marchand*, A. D. Laurent, Z. Chen, O. Siri and D. Jacquemin*
The Exceptional Stability of Azacalixphyrin and its Dianion
J. Phys. Chem. A (IF=2.693), **118** (2014) 8883–8888 doi.

284. A.Lietard, G. Piani, L. Poisson*, B. Soep, J. M. Mestdagh, S. Aloïse, A. Perrier, D. Jacquemin and M. Takeshita
Competitive Direct versus *Indirect Photochromism Dynamics in Constrained Inverse Dithienylethene Molecules*
Phys. Chem. Chem. Phys. (IF=4.493), **16** (2014) 22262–22272 doi.

285. A. D. Laurent* and D. Jacquemin*
Analyzing Excited-State Processes and Optical Signatures of a Ratiometric Fluorine Anion Sensor: a Quantum Look
Sc. China Chem. (IF=1.695), **57** (2014) 1363–1368 doi.

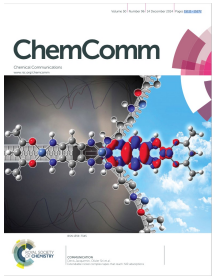
286. A. Charaf-Eddin, B. Le Guennic* and D. Jacquemin*
Excited-States of BODIPY-Cyanines: Ultimate TD-DFT Challenges ?
RSC Adv. (IF=3.840), **4** (2014) 49449–49456 doi.

287. P. Boulanger, S. Chibani, B. Le Guennic, I. Duchemin X. Blase* and D. Jacquemin*
Combining the Bethe-Salpeter Formalism with Time-Dependent DFT Excited-State Forces to Describe Optical Signatures: NBO Fluoroborates as Working Examples
J. Chem. Theory Comput. (IF=5.498), **10** (2014) 4548–4556 doi.

288. S. Chibani, A. D. Laurent*, B. Le Guennic* and D. Jacquemin*
Improving the Accuracy of Excited State Simulations of BODIPY and aza-BODIPY Dyes with a Joint SOS-CIS(D) and TD-DFT Approach
J. Chem. Theory Comput. (IF=5.498), **10** (2014) 4574–4582 doi.

289. B. Moore II, A. Charaf-Eddin, A. Planchat, C. Adamo, J. Autschbach* and D. Jacquemin*
Electronic Band Shapes Calculated with Optimally-Tuned Range-Separated Hybrid Functionals
J. Chem. Theory Comput. (IF=5.498), **10** (2014) 4599–4608 doi.

290. A. Charaf-Eddin, T. Cauchy, F.X. Felpin and D. Jacquemin*
Most Read Articles *Vibronic Spectra of Organic Electronic Chromophores*
RSC Adv. (IF=3.840), **4** (2014) 55466–55472 doi.



291. P. Hubin*, A. D. Laurent, D. P. Vercauteren and D. Jacquemin*
Investigation of ESIPT in a Panel Chromophores Presenting N-H...N Intramolecular Hydrogen Bonds
Phys. Chem. Chem. Phys. (IF=4.493), **16** (2014) 25288–25295 doi.

292. H. Audi, Z. Chen, A. Charaf-Eddin, A. D'aléo, G. Canard, D. Jacquemin* and O. Siri*
Extendable Nickel Complex Tapes
Chem. Comm. (IF=6.834), **50** (2014) 15140–15143 doi.

293. K. Benelhadj, J. Massue*, P. Retailleau, S. Chibani, B. Le Guennic, D. Jacquemin,* G. Ulrich* and R. Ziessel*
Solution- and Solid-State Luminescent Borate Complexes Based on a Substituted Π*-Conjugated 2-(2'-hydroxybenzofuran) Scaffold*
Eur. J. Org. Chem. (IF=3.065), (2014) 7156–7164 doi.

294. S. Chibani, S. Budzak, M. Medved, B. Mennucci* and D. Jacquemin*
Full cLR-PCM Calculations of the Solvatochromic Effects on Emission Energies
Phys. Chem. Chem. Phys. (IF=4.493), **16** (2014) 26024–26029 doi.

295. S. Aloïse*, R. Yibin, H. Ismail, G. Buntinx, A. Perrier*, F. Maurel, D. Jacquemin* and M. Takeshita
The Photochemistry of Inverse Dithienylethene Switches Understood
Phys. Chem. Chem. Phys. (IF=4.493), **16** (2014) 26762–26768 doi.

296. T. Jaunet-Lahary, A. Chantzis*, K. J. Chen, A. D. Laurent and D. Jacquemin*
Designing Efficient Azobenzene and Azothiophene Nonlinear Optical Photochromes
J. Phys. Chem. C (IF=4.772), **118** (2014) 28831–28841 doi.

297. U. Bussy, U. Jurva, R. Boisseai, M. Andresen-Bergström, V. Silvestre, N. Galland, D. Jacquemin and M. Boujtita*
Unexpected Benzimidazol Ring Formation from Quinoneimide Species in the Presence of Ammonium Acetate as Supporting Electrolyte Used in the Coupling Electrochemistry with Mass Spectrometry
Rapid Commun. Mass Spectrom. (IF=2.226), **29** (2015) 456–460 doi.

298. A. Maufroy, L. Favereau, F. B. Anne, Y. Pellegrin, E. Blart, M. Hissler, D. Jacquemin* and F. Odobel*
Synthesis and Properties of Push-Pull Porphyrins as Sensitizers for NiO Based Dye-Sensitized Solar Cells
J. Mater. Chem. A (IF=8.262), **3** (2015) 3908–3917 doi – errata **3** (2015) 6686–6686 doi

299. G. Marchand*, H. Roy, D. Mendive-Tapia and D. Jacquemin*
N-Confused Porphyrin Tautomers: Lessons from Density Functional Theory
Phys. Chem. Chem. Phys. (IF=4.449), **17** (2015) 5290–5297 doi.

300. Y. Houari, S. Chibani, D. Jacquemin and A. D. Laurent*
A TD-DFT Assessment of the Excited State Intramolecular Proton Transfer in HydroxyphenylBenzImidazole (HBI) Dyes
J. Phys. Chem. B (IF=3.187), **119** (2015) 2180–2192 doi.

301. C. Laurence*, J. Legros, A. Chantzis, A. Planchat and D. Jacquemin
A Database of Dispersion-Induction DI, Electrostatic ES, and Hydrogen Bonding α_1 *and* β_1 *Solvent Parameters and Some Applications*
J. Phys. Chem. B (IF=3.187), **119** (2015) 3174–3184 doi.

302. K. J. Chen, A. Charaf-Eddin, B. Selvam, F. Boucher, A. D. Laurent and D. Jacquemin*
Interplay Between TiO_2 *Surface and Organic Photochromes: A DFT Study Of Adsorbed Azobenzenes and Diarylethenes*
J. Phys. Chem. C (IF=4.509), **119** (2015) 3684–3696 doi.

303. T. Jaunet-Lahary, D. Jacquemin, B. Legouin, J. Y. Le Questel, J. F. Cupif, L. Toupet, P. Uriac* and J. Graton*
Dissymmetric Molecular Tweezers in Host-Guest Complexes: Internal or External Complexation ?
J. Phys. Chem. C (IF=4.509), **119** (2015) 3771–3779 doi.

304. B. Mennucci, G. Scalmani and D. Jacquemin*
Excited-State Vibrations of Solvated Molecules: Going Beyond the Linear-Response Polarizable Continuum Model
J. Chem. Theory Comput. (IF=5.301), **11** (2015) 847–859 doi.

305. J. P. Ceron-Carrasco*, A. Requena, J. Zuniga and D. Jacquemin
Mutagenic Effects Induced by the Attack of NO_2 Radical to the Guanine-Cytosine Base Pair
Front. Chem. (IF=N/A), **3** (2015) 13 (7p) doi.

306. J. P. Ceron-Carrasco* and D. Jacquemin
chemistryworld *DNA Spontaneous Mutation and its Role in the Evolution of GC-Content: Assessing the Impact of the Genetic Sequence*
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307. B. Le Guennic* and D. Jacquemin*
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Acc. Chem. Res. (IF=22.003), **48** (2015) 530–537 doi.

308. M. Medved*, S. Budzak, A. Laurent and D. Jacquemin
Direct and Indirect Effects of Dispersion Interactions on the Electric Properties of Weakly Bounded Complexes
J. Phys. Chem. A (IF=2.883), **119** (2015) 3112–3124 doi.

309. J. Boixel, V. Guerchais*, H. Le Bozec, A. Chantzis, D. Jacquemin*, A. Colombo*, C. Dragonetti, S. Righetto and D. Roberto*
Sequential Double Second-Order Nonlinear Optical Switch by an Acido-Triggered Photochromic Cyclometallated Platinum(II) Complex
Chem. Comm. (IF=6.567), **51** (2015) 7805–7808 doi.

310. D. Escudero* and D. Jacquemin
Computational insights into the photodeactivation dynamics of phosphors for OLEDs: a Perspective
Dalton Tans. (IF=4.177), *perpsective*, **44** (2015) 8346–8355 doi.

311. A. Fihey and D. Jacquemin*
Designing Efficient Photochromic Dithienylethene Dyads
Chem. Sci. (IF=9.144), **6** (2015) 3495–3503 doi.

312. A. D. Laurent, A. Blondel and D. Jacquemin*
Choosing an Atomic Basis Set for TD-DFT, SOPPA, ADC(2), CIS(D), CC2 and EOM-CCSD Calculations of Low-Lying Excited-States of Organic Dyes
Theor. Chem. Acc. (IF=1.806), **134** (2015) 76 (11p) doi.

313. S. Chibani, A. D. Laurent, B. Le Guennic* and D. Jacquemin*
Excited States of Ladder-Type π-conjugated Dyes with a Joint SOS-CIS(D) and PCM-TD-DFT Approach
J. Phys. Chem. A (IF=2.883), **119** (2015) 5417–5425 doi.

314. A. Fihey, A. Perrier, W. R. Browne and D. Jacquemin*
Most Read Articles *Multiphotochromic Molecular Systems*
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315. S. Ji,* J. Ge, D. Escudero, Z. Wang, J. Zhao,* and D. Jacquemin*
Molecular Structure-Intersystem Crossing Relationship of Heavy Atom-Free BODIPY Triplet Photosensitizers
J. Org. Chem. (IF=4.785), **80** (2015) 5958–5963 doi.

316. A. Felouat, A. D'Aléo, A. Charaf-Eddin, D. Jacquemin, B. Le Guennic⋆, E. Kim, K. J. Lee, J. H. Woo, J.C. Ribierre, J. W. Wu⋆ and F. Fages⋆
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Most Read Articles J. Chem. Theory Comput. (IF=5.301), **11** (2015) 3290–3304 doi.

318. K. J. Chen, F. Boucher and D. Jacquemin⋆
How Adsorption onto TiO_2 Modifies the Properties of Multi-Switchable DTE Systems: Theoretical Insights
J. Phys. Chem. C (IF=4.509), **119** (2015) 16860–16869 doi.

319. A. Fihey⋆, B. Le Guennic and D. Jacquemin⋆
Toward an Enhancement of the Photoactivity of Multiphotochromic Dimers Using Plasmon Resonance: a Theoretical Study
J. Phys. Chem. Lett. (IF=8.539), **6** (2015) 3067–3073 doi – errata: **6** (2015) 3366–3366 doi.

320. M. Frigoli⋆, J. Marrot, P. L. Gentili, D. Jacquemin⋆ M. Vagnini, D. Pannacci and F. Ortica⋆
P-type Photochromism of new Helical Chromenes: Synthesis, Photochemical, Photophysical and Theoretical Study
ChemPhysChem (IF=3.138), **16** (2015) 2447–2458 doi.

321. X. D. Jiang⋆, D. Xi, B. Le Guennic⋆, J. Guan, D. Jacquemin, J. Guan and and L. J. Xiao
Synthesis of the NIR Naphthyl-Containing aza-BODIPY and Measure of the Singlet Oxygen Generation
Tetrahedron (IF=2.645), **71** (2015) 7676–7680 doi.

322. B. Lasorne⋆, A. Fihey, D. Mendive-Tapia and D. Jacquemin⋆
A Curve-Crossing Model to Rationalize and Optimize Diarylethene Dyads
Chem. Sci. (IF=9.144), **6** (2015) 5695–5702 doi.

323. S. Maione, A. Gil, G. Fabregat, L. J. del Valle, J. Triguero, A. D. Laurent, D. Jacquemin, F. Extrany, D. Zanuy, C. Cativela⋆ and C. Aleman⋆
Electroactive Polymer-Peptide Conjugates for Adhesive Biointerfaces
Biomater. Sci. (IF=3.614), **3** (2015) 1395–1405 doi.

324. D. Ameline, S. Diring, Y. Farre, Y. Pellegrin, G. Naponiello, E. Blart, B. Charrier, D. Dini, D. Jacquemin⋆ and F. Odobel⋆
Isoindigo Derivatives for Application in p-Type Dye Sensitized Solar Cells
RSC Adv. (IF=3.289), **5** (2015) 85530–85539 doi.

325. K. Xu, J. Zhao⋆, D. Escudero, Z. Mahmood and D. Jacquemin⋆
Controlling Triplet-Triplet Annihilation Upconversion by Tuning the PET and ISC of Aminomethyleneanthracene Derivatives
J. Phys. Chem. C (IF=4.509), **119** (2015) 23801–23812 doi.

326. D. Jacquemin⋆, I. Duchemin and X. Blase⋆
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327. J. P. Ceron-Carrasco⋆ and D. Jacquemin⋆
Photoactivatable Platinum(II) Compounds: in Search of Novel Anticancer Drugs
Theor. Chem. Acc. (IF=1.806), **134** (2015) 146 (8p) doi.

328. V. Riffet, D. Jacquemin and G. Frison⋆
H-Atom Loss and Migration in Hydrogen-Rich Peptide Cation Radicals: The Role of Chemical Environment
Int. J. Mass Spectrom. (IF=2.183), **390** (2015) 28–38 doi.

329. C. A. Guido,⋆ D. Jacquemin, C. Adamo and B. Mennucci⋆
Most Read Articles
Electronic Excitations in Solution: The Interplay between State Specific Approaches and a TD-DFT Description
J. Chem. Theory Comput. (IF=5.301), **11** (2015) 5782–5790 doi.

330. G. Marchand⋆, J. C. Soetens, D. Jacquemin and P. A. Bopp
Effect of the Cation Model on the Dynamics of Poly-L-glutamate in Aqueous Sodium Chloride Solution
J. Chem. Phys. (IF=2.894), **143** (2015) 224505 (11p) doi.

331. S. Budzak, A. Charaf-Eddin, M. Medved, D. T. Gryko and D. Jacquemin⋆
Optical Properties of V-shaped Bis-Coumarins: Ab initio Insights
Comput. Theor. Chem. (IF=1.549), **1076** (2016) 57–64 doi.

332. P. O. Hubin,⋆ L. Leherte, D. Jacquemin and D. P. Vercauteren
Accessing the Free Energy Profile of an Organic Reaction by Using a Reactive Force Field
Theor. Chem. Acc. (IF=1.890), **135** (2016) 16 (10p) doi.

333. E. Kim, A. Felouat, E. Zaborova, J. C. Ribierre, J. W. Wu, S. Senatore, C. Matthews, P. F. Lenne, C. Baffert, A. Karapetyan, M. Giorgi, D. Jacquemin, M. A. Ponce-Vargas, B. Le Guennic, F. Fages and A. D'Aleo⋆
Boron Difluoride Complexes of Hemicurcuminoids as Bio-inspired Push-Pull Dyes for Bioimaging
Org. Biomol. Chem. (IF=3.564), **14** (2016) 1311–1324 doi.

334. J. P. Ceron-Carrasco⋆, D. Jacquemin⋆ and A. D. Laurent⋆
First Computational Step Towards the Understanding of the Antioxidant Activity of the Phycocyanobilin:Ferredoxin Oxidoreductase in Complex with Biliverdin IXα
Comput. Theor. Chem. (IF=1.549), **1077** (2016) 58–64 doi.

335. K. J. Chen, A. D. Laurent, F. Boucher, F. Odobel and D. Jacquemin⋆
Determining the Most Promising Anchors for CuSCN: Ab Initio Insights towards p-Type DSSCs
J. Mater. Chem. A (IF=8.867), **4** (2016) 2217–2227 doi.

336. L. Dondaine, D. Escudero, M. Ali, P. Richard, F. Denat, A. Bettaieb, P. Le Gendre, C. Paul, D. Jacquemin,⋆ C. Goze⋆ and E. Bodio⋆
Coumarin-Phosphine-Based Smart Probes for Tracking Biological Relevant Metal Complexes: from Theoretical to Biological Investigations
Eur. J. Inorg. Chem. (IF=2.444), (2016) 545–553 doi.

337. A. Grabarz, A. D. Laurent, B. Jedrzejewska, A. Zakrzewska, D. Jacquemin⋆ and B. Osmialowski⋆
The Influence of the π-Conjugated Spacer on Photophysical Properties of (Di)fluoroboranyls Derived from Amides Carrying Donor Group
J. Org. Chem. (IF=4.849), **81** (2016) 2280–2292 doi.

338. R. Beneteau, A. Boussonniere, J. C. Rouaud, J. Lebreton, J. Graton, D. Jacquemin, M. Sebban, H. Oulyadi, G. Hamdoun, A. N. Hancock, C. H. Schiesser and F. Denes⋆
Radical Cyclization of α-Halo Aluminium Acetals: A Mechanistic Study
Chem. Eur. J. (IF=5.317), **22** (2016) 4809–4824 doi.

339. A. Fihey, A. Favennec, B. Le Guennic⋆ and D. Jacquemin⋆
Investigating the properties of PODIPY (Phosphorous-Dipyrromethene) with ab initio tools
Phys. Chem. Chem. Phys. (IF=4.123), **18** (2016) 9358–9366 doi.

340. G. Marchand⋆, P. Giraudeau, Z. Chen, O. Siri⋆ and D. Jacquemin⋆
Understanding Tautomerism in Azacalixphyrins
Phys. Chem. Chem. Phys. (IF=4.123), **18** (2016) 9608–9615 doi.

341. K. Kamada⋆, T. Namikawa, S. Senatore, C. Matthews, P. F. Lenne, O. Maury, C. Andraud, M. A. Ponce Vargas, B. Le Guennic, D. Jacquemin, P. Agbo, D. D. An, S. S. Gauny, X. Liu, R. J. Abergel⋆, F. Fages and A. D'Aleo⋆
Borondifluoride Curcuminoid Fluorophores with Enhanced Two-Photon Excited Fluorescence Emission and Versatile Living-Cell Imaging Properties
Chem. Eur. J. (IF=5.317), **22** (2016) 5219–5232 doi.

342. S. Budzak, A. D. Laurent, C. Laurence, M. Medved and D. Jacquemin*
Solvatochromic Shifts in UV-Vis Absorption Spectra: The Challenging Case of 4-Nitropyridine N-Oxide
J. Chem. Theory Comput. (IF=5.245), **12** (2016) 1919–1929 doi.

343. D. Jacquemin*, I. Duchemin and X. Blase*
Assessment of the Convergence of Partially Self-Consistent BSE/GW Calculations
Mol. Phys. (IF=1.870), **114** (2016) 957–967 doi.

344. Y. Farre, L. Zhang, Y. Pellegrin, A.Planchat, E. Blart, M. Boujtita, L. Hammarstrom*, D. Jacquemin* and F. Odobel*
Second Generation of Diketopyrrolopyrrole Dyes for NiO Based Dye-Sensitized Solar Cells
J. Phys. Chem. C (IF=4.536), **120** (2016) 7923–7940 doi.

345. P. Le Pogam, A.-C. Le Lamer, S. Bandi, B. Legouin, A. Bondon, J. Graton, D. Jacquemin, P. Uriac, I. Rouaud, S. Ferron, W. Obermayer, K. Suresh Babu and J. Boustie*
Minor Naphthazarinopyranones from Lichen Ophioparma Ventosa Apotheciae
J. Nat. Prod. (IF=3.281), **79** (2016) 1005–1011 doi.

346. I. Duchemin*, D. Jacquemin and X. Blase
Combining the GW Formalism with the Polarizable Continuum Model : a State-Specific Non-Equilibrium Approach
J. Chem. Phys. (IF=2.965), **144** (2016) 164106 (13 p) doi.

347. E. Hitti, B. Legouin, J. Graton, D. Jacquemin and P. Uriac*
^{1}H NMR and Computational Studies of the Conformations in Solution of one Host/Guest Complex Formed with an Usnic Acid Tweezer and 2,4,7-Trinitro-9-fluorenone (TNF)
Tetrahedron (IF=2.651), **72** (2016) 2890–2894 doi.

348. C. Azarias and D. Jacquemin*
Elucidating the Nature of Carbazole-Porphyrinoids with First-Principle Approaches
J. Phys. Chem. A (IF=2.847), **120** (2016) 2824–2831 doi.

349. S. Pascal, C. Besnard, F. Zinna, L. Di Bari, B. Le Guennic, D. Jacquemin and J. Lacour*
Zwitterionic [4]Helicene: a Water-Soluble and Reversible pH Triggered ECD/CPL Chiroptical Switch in the UV and Red Spectral Regions
Org. Biomol. Chem. (IF=3.564), **14** (2016) 4590–4594 doi.

350. W. Yang, J. Zhao,* C. Sonn, D. Escudero, A. Karatay, H. G. Yaglioglu, B. Küçüköz, M. Hayvali,* C. Li,* and D. Jacquemin*
Efficient Intersystem Crossing in Heavy atom-Free Perylenebisimide Derivatives
J. Phys. Chem. C (IF=4.536), **120** (2016) 10162–10175 doi.

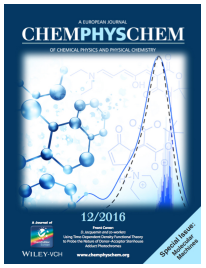
351. C. Azarias, S. Budzak, A. D. Laurent, G. Ulrich and D. Jacquemin*
Tuning ESIPT Fluorophores into Dual Emitters
Chem. Sci. (IF=8.668), **7** (2016) 3763–3774 doi.

352. A. Fihey* and D. Jacquemin*
How Metals Can Help Multiphotochromism: an Ab Initio Study
J. Phys. Chem. C (IF=4.536), **120** (2016) 11140–11150 doi.

353. M. C. Chang, A. Chantzis, D. Jacquemin and E. Otten*
Boron Difluorides with Formazanate Ligands: Redox-Switchable Fluorescent Dyes with Large Stokes Shifts
Dalton Trans. (IF=4.029), **45** (2016) 9477–9484 doi.

354. M. d'Halluin, J. Rull-Barrull, E. Le Grognec, D. Jacquemin and F.X. Felpin*
Writing and Erasing Hidden Optical Information on Covalently Modified Cellulose Paper
Chem. Comm. (IF=6.319), **52** (2016) 7672–7675 doi.

355. A. Prlj, M. E. Sandoval-Salinas, D. Casanova, D. Jacquemin* and C. Corminboeuf*
Most Read Articles
Low Lying $\pi\pi^*$ States of Heteroaromatic Molecules: A Challenge for Excited State Methods
J. Chem. Theory Comput. (IF=5.245), **12** (2016) 2652–2660 doi.



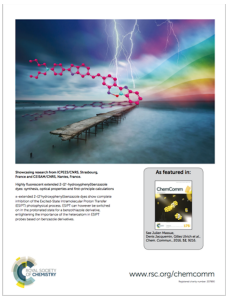
VIP

356. A.D. Laurent, M. Medved' and D. Jacquemin⋆
Using TD-DFT to Probe the Nature of Donor-Acceptor Stenhouse Adduct Photochromes
ChemPhysChem (IF=3.075), **17** (2016) 1846–1851 doi.

357. B. Jedrzejewska, A. Zakrzewska, G. Mloston, S Budzak, K. Mroczynska, A. M. Grabarz, M. Kaczorowska, D. Jacquemin and B. Osmialowski⋆
Synthesis and Photophysical Properties of Novel Donor-Acceptor N-(Pirydyn-2-yl) Substituted Benzo(thio)amides and their Difluoroboranyl Derivatives
J. Phys. Chem. A (IF=2.847), **120** (2016) 4116–4123 doi.

358. A. D. Laurent, B. Le Guennic and D. Jacquemin⋆
Theoretical Spectroscopy of BASHY Dyes
Theor. Chem. Acc. (IF=1.890), **135** (2016) 173 (8p) doi.

359. S. Budzak and D. Jacquemin⋆
Mechanism of Fluorescence Switching in one ESIPT-Based Al^{3+} Probe
J. Phys. Chem. B (IF=3.177), **120** (2016) 6730–6738 doi.



360. M. Raoui, J. Massue⋆, C. Azarias, D. D. Jacquemin⋆ and G. Ulrich⋆
Highly Fluorescent Extended 2-(2'Hydroxyphenyl)Benzazole Dyes: Synthesis, Optical Properties and First-Principle Calculations
Chem. Comm. (IF=6.319), **52** (2016) 9216–9219 doi.

361. S. Nishizawa, A. Fihey, D. Jacquemin⋆ and K. Matsuda⋆
Computational Investigation on the Switching Efficiency of Diarylethene: Comparison Between the First Hyperpolarizability and Exchange Interaction
Chem. Phys. Lett. (IF=1.815), **659** (2016) 258–262 doi.

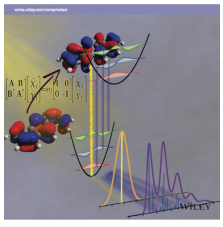
362. J. Boixel⋆, Y. Zhu, H. Le Bozec, M. A. Benmensour, A. Boucekkine, K. Man-Chung Wong, A. Colombo, D. Roberto, V. Guerchais⋆ and D. Jacquemin⋆
Contrasted Photochromic and Luminescent Properties in Dinuclear Pt(II) Complexes Linked Through a Central DTE Unit
Chem. Comm. (IF=6.319), **52** (2016) 9833–9836 doi.

363. T. Jaunet-Lahary, A. Goupille, D. Jacquemin, F. Fleury, J. Graton⋆ and A. D. Laurent⋆
A Joint Theoretical and Experimental Study of the Behavior of the DIDS Inhibitor and its Derivatives
ChemPhysChem (IF=3.075), **17** (2016) 2434–2445 doi.

364. D. Jacquemin⋆, I. Duchemin, A. Blondel and X. Blase⋆
Assessment of the Accuracy of the Bethe-Salpeter (BSE/GW) Oscillator Strengths
J. Chem. Theory Comput. (IF=5.245), **12** (2016) 3969–3981 doi.

Most Read Articles

365. D. Jacquemin⋆
Excited-State Dipole and Quadrupole Moments: TD-DFT versus CC2
J. Chem. Theory Comput. (IF=5.245), **12** (2016) 3993–4003 doi.



366. F. Santoro⋆ and D. Jacquemin⋆
Going Beyond the Vertical Approximation with TD-DFT
WIREs Comp. Mol. Sc. (IF=14.016), **6** (2016) 460–486 doi.

367. D. S. Andrianov, Y. Farré, K. J. Chen, A. Planchat, D. Jacquemin⋆, A. V. Cheprakov⋆ and F. Odobel⋆
Trans-Substituted Benzodiazaporphyrin: a Promising Hybrid Dye Between Porphyrin and Phthalocyanine for Application in Dye-Sensitized Solar Cells
J. Photochem. Photobiol. A: Chem. (IF=2.625), **330** (2016) 186–194 doi.

368. L. Zhang, L. Favereau, Y. Farré, A. Maufroy, Y. Pellegrin, E. Blart, M. Hissler, D. Jacquemin, F. Odobel⋆ and L. Hammarström⋆
Molecular-Structure Control of Electron Transfer Dynamics of Push-Pull Porphyrins as Sensitizer for NiO Based Dye Sensitized Solar Cells
RSC Adv. (IF=3.108), **6** (2016) 77184–77194 doi.

369. A. Belhboub, F. Boucher and D. Jacquemin*
Grafting Spiropyran Molecular Switches on TiO_2: A First-Principles Study
J. Phys. Chem. C (IF=4.536), **120** (2016) 18281–18288 doi.

370. P. O. Hubin*, D. Jacquemin, L. Leherte and D. P. Vercauteren
Parameterization of the ReaxFF Reactive Force Field for a Proline-Catalyzed Aldol Reaction
J. Comput. Chem. (IF=3.229), **37** (2016) 2564–2572 doi.

371. R. Russo, A. Fihey, B. Mennucci* and D. Jacquemin*
Theoretical Quantification of the Modified Photoactivity of Photochromes Grafted on Metallic Nanoparticles
J. Phys. Chem. C (IF=4.536), **120** (2016) 21827–21836 doi.

372. G. Marchand*, O. Siri and D. Jacquemin*
Effects of Chemical Substitutions on the Properties of Azacalixphyrins: a First-principles Study
Phys. Chem. Chem. Phys. (IF=4.123), **18** (2016) 27308–27316 doi.

373. T. T. Dang, J. F. Soulé, H. Doucet, M. A. Benmensour, A. Boucekkine, A. Colombo*, C. Dragonetti, S. Righetto, D. Jacquemin, J. Boixel* and V. Guerchais
Asymmetrical 1,3-Bis-(Heteroazolyl)Benzene Platinum Complexes 2,3 with Tunable Second-Order Nonlinear Optical Properties
Eur. J. Inorg. Chem. (IF=2.444), (2016) 4774–4782 doi.

374. A. D. Laurent, E. Otten, B. Le Guennic* and D. Jacquemin*
Formazanate Boron Difluoride Dyes: Discrepancies Between TD-DFT and Wavefunction Descriptions
J. Mol. Model. (IF=1.425), **22** (2016) 263 (8p) doi.

375. D. Rota Martir, G. J. Hedley, D. B. Cordes, A. M. Z. Slawin, D. Escudero, D. Jacquemin, T. Kosikova, D. Philp, D. M. Dawson, S. E. Ashbrook, I. D. W. Samuel and E. Zysman-Colman*
Exploring the Self-Assembly and Energy Transfer of Dynamic Supramolecular Iridium-Porphyrin Systems
Dalton Trans. (IF=4.029), **45** (2016) 17195–17205 doi.

376. D. B. Zhang, J. Y. Wang, D. Jacquemin and Z. N. Chen*
Spectroscopic and Electrochemical Properties of Ruthenium Complexes with Photochromic Triarylamine-Dithienylethene-Acetylide Ligands
Inorg. Chem. Front. (IF=4.036), **3** (2016) 1432–1443 doi.

377. D. Mendive-Tapia*, L. Kortekaas, J. D. Steen, A. Perrier, B. Lasorne, W. R. Browne* and D. Jacquemin*
Accidental Degeneracy in the Spiropyran Radical Cation: Charge Transfer Between two Orthogonal Rings Inducing Ultra-Efficient Reactivity
Phys. Chem. Chem. Phys. (IF=4.123), **18** (2016) 31244–31253 doi.

378. Z. Chen, R. Haddoub, J. Mahé, G. Marchand, D. Jacquemin*, J. Andeme-Edzang, G. Canard, D. Ferry, O. Grauby, A. Ranguis and O. Siri*
N-Substituted Azacalixphyrins: Synthesis, Properties and Self-assembly
Chem. Eur. J. (IF=5.317), **22** (2016) 17820–17832 doi.

379. X. D. Jiang*, S. Li, B. Le Guennic*, D. Jacquemin, D. Escudero and L. J. Xiao
Singlet Oxygen Generation Properties of Isometrical Dibromated Thienyl-Containing Aza-BODIPYs
Phys. Chem. Chem. Phys. (IF=4.123), **18** (2016) 32686–32690 doi.

380. J. Bosson, G. M. Labrador, S. Pascal, F. A. Miannay, O. Yushchenko, H. Li, L. Bouffier, N. Sojic, R. C. Tovar, G. Muller, D. Jacquemin, A. D. Laurent, B. Le Guennic, E. Vauthey* and J. Lacour*
Most Accessed
Physicochemical and Electronic Properties of Cationic [6]Helicenes, from Chemical and Electrochemical Stabilities to Far-Red (Polarized) Luminescence
Chem. Eur. J. (IF=5.317), **22** (2016) 18394–18403 doi; Err: *ibidem*, **25** (2019) 1.

381. X. D. Jiang⋆, J. Guan, J. Zhao, B. Le Guennic⋆, D. Jacquemin, Z. Zhang, S. Chena and L. J. Xiao
Synthesis, Structure and Photophysical Properties of NIR aza-BODIPYs with -F/-N_3/-NH_2 at 1,7-Positions
Dyes Pigm. (IF=3.767), **136** (2017) 619–626 doi.

382. F. Bassal, A. D. Laurent, B. Le Guennic and D. Jacquemin⋆
Exploring the Excited-States of Squaraine Dyes with TD-DFT, SOS-CIS(D) and ADC(2)
Dyes Pigm. (IF=3.767), **138** (2017) 169–175 doi.

383. S. Pascal, S. Denis-Quanquin, C. Monnereau, A. Duperray, A. Grichine, B. Le Guennic, D. Jacquemin, J. Cuny, S. H. Chi, J. W. Perry, F. Appaix, B. van der Sanden, C. Andraud⋆ and O. Maury⋆
Keto-Polymethines: a Versatile Class of Dyes with Outstanding Spectroscopic Properties for In Cellulo and In Vivo Two-Photon Microscopy Imaging
Chem. Sci. (IF=9.556), **8** (2017) 381–394 doi.

384. A. Fihey⋆, R. Russo, L. Cupellini, D. Jacquemin⋆ and B. Mennucci⋆
Is Energy Transfer Limiting Multiphotochromism ? Answers from ab initio *Quantification*
Phys. Chem. Chem. Phys. (IF=3.906), **19** (2017) 2044–2052 doi.

385. C. Azarias, I. Duchemin, X. Blase and D. Jacquemin⋆
Bethe-Salpeter Study of Cationic Dyes: Comparisons with ADC(2) and TD-DFT
J. Chem. Phys. (IF=2.997), **146** (2017) 034301 (8p) doi.

386. D. Gao, C. Azarias, A. D'Aléo, M. Giorgi, O. Siri, T. S. Balaban, D. Jacquemin⋆ and G. Canard⋆
Synthesis and Characterization of Phophorus meso*-Ester Corroles*
Eur. J. Inorg. Chem. (IF=2.507), (2017) 780–788 doi.

387. G. Zhang, D. Jacquemin⋆ and D. Buccella⋆
Tuning the Spectroscopic Properties of Ratiometric Fluorescent Metal Indicators: Experimental and Computational Studies on Mag-fura-2 and Analogues
J. Phys. Chem. B (IF=2.923), **121** (2017) 696–705 doi.

388. A. M. Grabarz, B. Jedrzejewska, A. Zakrzewska, R. Zalesny, A. D. Laurent, D. Jacquemin⋆ and B. Osmialowski⋆
Photophysical Properties of Phenacylphenantridine Difluoroboranyls: Effect of Substituent and Double Benzannulation
J. Org. Chem. (IF=4.745), **82** (2017) 1529–1537 doi.

389. G. Canard⋆, M. Ponce-Vargas, D. Jacquemin, B. Le Guennic⋆, A. Felouat, E. Zaborova, A. D'Aléo and F. Fagès⋆
Influence of the Electron Donor Groups on the Optical and Electrochemical Properties of Borondifluoride Complexes of Curcuminoid Dderivatives: a Joint Theoretical and Experimental Study
RSC Adv. (IF=2.936), **7** (2017) 10132–10142 doi.

390. A. Garcia, P. R. Pratap, C. Lüpfert, F. Cornelius, D. Jacquemin, B. Levg, T. W. Alleng and R. J. Clarke⋆
The Voltage-Sensitive Dye RH421 Detects a Na^+,K^+-ATPase Conformational Change at the Membrane Surface
BBA Biomembranes (IF=3.438), **1859** (2017) 813–823 doi.

391. D. Jacquemin⋆, I. Duchemin, A. Blondel and X. Blase⋆
Benchmark of Bethe-Salpeter for Triplet Excited-States
J. Chem. Theory Comput. (IF=5.313), **13** (2017) 767–783 doi.

392. D. Escudero, I. Duchemin, X. Blase and D. Jacquemin⋆
Modelling the Photochrome-TiO_2 Interface with Bethe-Salpeter and TD-DFT Methods
J. Phys. Chem. Lett. (IF=7.329), **8** (2017) 936–940 doi.

393. D. Rota Martir, M. Averardi, D. Escudero, D. Jacquemin and E. Zysman-Colman⋆
Photoinduced Electron Transfer in Supramolecular Ruthenium-Porphyrin Assemblies
Dalton Trans. (IF=4.052), **46** (2017) 2255–2262 doi.

394. A. Belhboub, F. Boucher, and D. Jacquemin*
Ab Initio Investigation of Photoswitches Adsorbed onto Metal Oxide Surfaces: The Case of Donor-Acceptor Stenhouse Adduct Photochromes on TiO_2 Anatase
J. Mater. Chem. C (IF=6.641), **5** (2017) 1624–1631 doi.

395. C. Azarias, R. Russo, L. Cupellini, B. Mennucci* and D. Jacquemin*
Modeling Excited-State Energy Transfer in Multi-BODIPY Architectures
Phys. Chem. Chem. Phys. (IF=3.906), **19** (2017) 6443–6453 doi.

396. B. Stefane*, F. Pozgan, E. Kim, E. Choi, J. C. Ribierre, J. W. Wu, M. Ponce-Vargas, B. Le Guennic*, D. Jacquemin, G. Canard, E. Zaborova, F. Fages* and A. D'Aléo*
Ethynylene-Analogues of Hemicurcuminoids: Synthesis and Ground- and Excited Properties of their Boron Difluoride Complexes
Dyes Pigm. (IF=3.767), **141** (2017) 38–47 doi.

397. R. Travieso-Puente, S. Budzak, J. Chen, P. Stacko, J. T. B. H. Jastrzebski, D. Jacquemin* and E. Otten*
Arylazoindazole Photoswitches : Facile Synthesis and Functionalization via S_N-Ar Substitution
J. Am. Chem. Soc. (IF=14.357), **139** (2017) 3328–3331 doi.

398. Y. M. Poronik, M. Mazur, M. Samoc*, D. Jacquemin* and D. T. Gryko*
2,5-Bis(azulenyl)pyrrolo[3,2-b]pyrroles – the Key Influence of the Linkage Position on the Linear and Non-Linear Optical Properties
J. Mater. Chem. C (IF=6.641), **5** (2017) 2620–2628 doi.

399. D. Jacquemin*, I. Duchemin, and X. Blase*
Is Bethe-Salpeter Formalism Accurate for Excitation Energies ? Comparisons with TD-DFT, CASPT2 and EOM-CCSD
J. Phys. Chem. Lett. (IF=7.329), **8** (2017) 1524–1529 doi.

400. S. Budzak, T. Jaunet-Lahary, A. D. Laurent, C. Laurence, M. Medved and D. Jacquemin*
Exploring the Solvatochromism of Betaine 30 with Ab Initio Tools: From Accurate Gas Phase Calculations to Implicit and Explicit Solvation Models
Chem. Eur. J. (IF=5.160), **23** (2017) 4108–4119 doi.

401. J. P. Cerón-Carrasco* and D. Jacquemin
Exposing the G-Quadruplex to Electric Fields: the Role Played by Telomeres in the Propagation of DNA Errors
Phys. Chem. Chem. Phys. (IF=3.906), **19** (2017) 9358–9365 doi.

402. B. Le Guennic, G. Sclamani, M. J. Frisch, A. D. Laurent and D. Jacquemin*
Investigating the Optical Properties of BOIMPY Dyes with ab initio *Tools*
Phys. Chem. Chem. Phys. (IF=3.906), **19** (2017) 10554–10561 doi.

403. C. Hierlinger, T. Roisnel, D. B. Cordes, A. M. Z. Slawin, D. Jacquemin*, V. Guerchais* and E. Zysman-Colman*
An Unprecedented Family of Luminescent Iridium(III) Complexes Bearing A six-Membered Chelated Tridentate C^N^C *Ligand*
Inorg. Chem. (IF=4.700), **56** (2017) 5182–5188 doi.

404. A. F. Henwood, J. Webster, D. Cordes, A. M. Z. Slawin, D. Jacquemin* and E. Zysman-Colman*
Phosphorescent Platinum(II) Complexes Bearing Pentafluorosulfanyl Substituted Cyclometalating Ligands
RSC Adv. (IF=2.936), **7** (2017) 25566–25574 doi.

405. C. A. Guido*, G. Sclamani, B. Mennucci and D. Jacquemin
Excited State Gradients for a State-Specic Continuum Solvation Approach: the Vertical Excitation Model within a Lagrangian TDDFT formulation
J. Chem. Phys. (IF=2.997), **146** (2017) 204106 (9 p) doi.

406. E. Heyer, K. Benelhadj, S. Budzak, D. Jacquemin*, J. Massue* and G. Ulrich*
On the Fine-Tuning of Excited-State Intramolecular Proton Transfer (ESIPT) Process in 2-(2'-Hydroxybenzofuran)benzazole (HBBX) Dyes
Chem. Eur. J. (IF=5.160), **23** (2017) 7324–7336 doi.

407. C. Azarias, M. Pawelek and D. Jacquemin*
Structural and Optical properties of Subporphyrinoids: a TD-DFT Study
J. Phys. Chem. A (IF=2.836), **121** (2017) 4306–4317 doi.

408. G. Marchand*, O. Siri and D. Jacquemin*
On the Structures, Spin States, and Optical Properties of Titanium, Platinum, and Iron Azacalixphyrins: A DFT Study
Phys. Chem. Chem. Phys. (IF=3.906), **19** (2017) 15903–15913 doi.

409. Y. Farré, M. Raissi, A. Fihey, Y. Pellegrin, E. Blart, D. Jacquemin* and F. Odobel*
A Blue Diketopyrrolopyrrole Sensitizer With High Efficiency in NiO Based Dye-Sensitized Solar Cells
ChemSusChem (IF=7.411), **10** (2017) 2618–2625 doi.

410. Z. Chen, G. Canard,* C. Azarias, D. Jacquemin* and O. Siri*
Straightforward Metal-Free Synthesis of an Azacalix[6]arene Forming a Host-Guest Complex with Fullerene C_{60}
New. J. Chem. (IF=3.201), **41** (2017) 5284–5290 doi.

411. J. Li, G. D'Avino*, A. Pershin, D. Jacquemin, I. Duchemin, D. Beljonne and X. Blase
Correlated Electron-Hole Mechanism for Molecular Doping in Organic Semiconductors
Phys. Rev. Mater. (IF=NA), **1** (2017) 025602 (9 p) doi.

412. L. G. Lukasiewicz, H. Gun Ryu, A. Mikhaylov, C. Azarias, M. Banasiewicz, B. Kozankiewicz*, K. Han Ahn*, D. Jacquemin*, A. Rebane* and D. G. Gryko*
Symmetry Breaking in Pyrrolo[3,2-b]pyrroles: Synthesis, Solvatofluorochromism and Two-photon Absorption
Chem. Asian J. (IF=3.692), **12** (2017) 1736–1748 doi.

413. A. Perrier* and D. Jacquemin*
Theoretical Investigation of the Photochromic Properties of [2.2]Paracyclophane-Bridged imidazole Dimers and Bis(imidazole) Dimers
Tetrahedron (IF=2.377), **73** (2017) 4936–4949 doi.

414. T. Biet, T. Cauchy, Q. sun, J. Ding, A. Hauser*, P. Oulevay, T. Bürgi, D. Jacquemin, N. Vanthuyne, J. Crassous and N. Avarvari*
Luminescent Helicene-Dithiolene Platinum Diimine Complexes
Chem. Comm. (IF=6.164), **53** (2017) 9210–9213 doi.

415. C. Azarias, C. Habert, S. Budzak, X. Blase, I. Duchemin and D. Jacquemin*
Calculations of $n \rightarrow \pi^*$ Transition Energies: Comparisons Between TD-DFT, ADC, CC, CASPT2 and BSE/GW Descriptions
J. Phys. Chem. A (IF=2.836), **121** (2017) 6122–6134 doi.

416. J. Bednarska*, R. Zalesny*, W. Bartkowiak, B. Ośmiałowski, M. Medved and D. Jacquemin*,
Quantifying the Performances of DFT for Predicting Vibrationally Resolved Optical Spectra: Asymmetric Fluoroborate Dyes as Working Examples
J. Chem. Theory Comput. (IF=5.313), **13** (2017) 4347–4356 doi.

417. W. Wang, B. Ashwood, J. Zhao*, W. Ji, D. Escudero*, D. Jacquemin* and C. Crespo-Hernandez*
Ultrafast Excited-State Dynamics in Cyclometalated Ir(III) Complexes Coordinated with Perylenebisimide and Its π-Radical Anions Ligands
J. Phys. Chem. C (IF=4.309), **121** (2017) 21184–21198 doi.

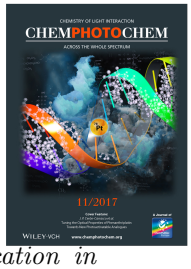
418. L. Lavaud, Z. Chen, M. Elhabiri, D. Jacquemin*, G. Canard and O. Siri*
Di- vs Tetra-Substituted Quinonediimines: a Drastic Effect in Coordination Chemistry
Dalton Trans. (IF=4.052), **46** (2017) 12794–12803 doi.

419. D. Rota Martir, D. Escudero, D. Jacquemin, D. B. Cordes, A. M. Z. Slawin, H. A. Fruchtl, S. L. Warriner and E. Zysman-Colman*
Homochiral Emissive Λ_8, Δ_8-$[Ir_8Pd_4]^{16+}$ Supramolecular Cages
Chem. Eur. J. (IF=5.160), **23** (2017) 14358–14366 doi.

420. D. Jacquemin and D. Escudero*
The Short Device Lifetimes of Blue PhOLEDs: Insights into the Photostability of Blue Ir(III) Complexes
Chem. Sci. (IF=9.556), **8** (2017) 7844–7850 doi.

421. C. Y. Huang, A. Bonasera, L. Hristov, Y. Garmashausen, B. M. Schmidt, D. Jacquemin* and S. Hecht*
N,N'-Disubstituted Indigos as Readily Available Red-Light Photoswitches with Tunable Thermal Half-Lives
J. Am. Chem. Soc. (IF=14.357), **139** (2017) 15205–15211 doi.

422. M. Di Donato, M. M. Lerch, A. Lapini, A. D. Laurent, A. Iagatti, L. Bussotti, S. P. Ihrig, M. Medved', D. Jacquemin, W. Szymanski, W. J. Jan Buma, P. Foggi and B. L. Feringa*
Shedding Light on the Photo-Isomerization Pathway of Donor-Acceptor Stenhouse Adducts
J. Am. Chem. Soc. (IF=14.357), **139** (2017) 15596–15599 doi.



423. J. P. Cerón-Carrasco* and D. Jacquemin
Tuning the Optical Properties of Phenanthriplatin: Towards new Photoactivatable Analogues
ChemPhotoChem (IF=NA), **1** (2017) 504–512 doi.

424. M. Ponce-Vargas*, C. Azarias, D. Jacquemin and B. Le Guennic
A Combined TD-DFT-SOS-CIS(D) Study of BOPHY Derivatives with Potential Application in Biosensing
J. Phys. Chem. B (IF=2.923), **121** (2017) 10850–10858 doi.

425. S. Budzak, G. Sclamani and D. Jacquemin*
Most Read Articles
Accurate Excited-State Geometries: a CASPT2 and Coupled-Cluster Reference Database for Small Molecules
J. Chem. Theory Comput. (IF=5.313), **13** (2017) 6237–6252 doi.

426. Y. Farré, M. Raissi, A. Fihey, Y. Pellegrin, E. Blart, D. Jacquemin* and F. Odobel*
Synthesis and Properties of New Benzothiadiazole-Based Push-Pull Dyes for P-Type Dye Sensitized Solar Cells
Dyes Pigm. (IF=4.018), **148** (2018) 154–166 doi.

427. E. Garoni, J. Boixel, V. Dorcet, T. Roisnel, D. Roberto, D. Jacquemin* and V. Guerchais*
Controlling the Emission in Flexibly-Linked (N^C^N)Platinum Dyads
Dalton Trans. (IF=4.052), **47** (2018) 224–232 doi.

428. C. Hierlinger, H. Flint, D. B. Cordes, A. M. Z. Slawin, E. A. Gibson*, D. Jacquemin*, V. Guerchais* and Eli Zysman-Colman*
A Panchromatic, Near Infrared Ir(III) Emitter Bearing a Tripodal C^N^C Ligand as a Dye for Dye-Sensitized Solar Cells
Polyhedron (IF=2.284), **140** (2018) 109–115 doi.

429. C. Azarias, L. Cupellini, A. Belhboub, B. Mennucci* and D. Jacquemin*
Modelling Excitation Energy Transfer in Covalently Linked Molecular Dyads Containing a BODIPY Unit and a Macrocycle
Phys. Chem. Chem. Phys. (IF=3.567), **20** (2018) 1993–2008 doi.

430. A. Colombo, R. Ossola, M. Magni, D. Roberto, D. Jacquemin, C. Castellano, F. Demartina* and C. Dragonetti*
Intriguing C-H···Cu Interactions in Bis-(Phenanthroline)Cu(I) Complexes: the First Example of an Anagostic Bond Between a Hydrogen Atom of a Methyl Group and Copper
Dalton Trans. (IF=4.052), **47** (2018) 1018–1022 doi.

431. X. Blase*, I. Duchemin and D. Jacquemin*
The Bethe-Salpeter Equation in Chemistry: Relations with TD-DFT, Applications and Challenges
Chem. Soc. Rev. (IF=40.443), **47** (2018) 1022–1043 doi.

432. M. Khelladi, N. Leclerc, D. Jacquemin, A. De Nicola* and G. Ulrich*
Synthesis and Spectral Properties of Orthogonal Red and Near IR Emitter DiBenzoBODIPYs
Tetrahedron Lett. (IF=2.259), **59** (2018) 878–881 doi.

433. C. Hierlinger, A. K. Pal, F. Stella, T. Lebl, D. B. Cordes, A. M. Z. Slawin, D. Jacquemin*, V. Guerchais* and E. Zysman-Colman*
Synthesis, Characterization and Optoelectronic Properties of Iridium Complexes Bearing Non-conjugated Six-membered Chelating Ligands
Inorg. Chem. (IF=4.850), **57** (2018) 2023–2034. doi.

434. F. Forato, A. Belhboub, J. Monot, M. Petit, R. Benoit, V. Sarou-Kanian, F. Fayon, D. Jacquemin, C. Queffelec* and B. Bujoli
Phosphonate-Mediated Immobilization of Rhodium/Bipyridine Hydrogenation Catalysts
Chem. Eur. J. (IF=5.160), **24** (2018) 2457–2465 doi.

435. K. Xu, A. A. Sukhanov, Y. Zhao, J. Zhao*, W. Ji, X. Peng, D. Escudero*, D. Jacquemin and V. K. Voronkova*
Unexpected Nucleophilic Substitution Reaction of Bodipy- TEMPO Triad : Radical Enhanced Intersystem Crossing, Electron Spin Polarization and Application for Triplet-Triplet Annihilation Upconversion
Eur. J. Org. Chem. (IF=3.029), (2018) 885–895 doi.

436. D. Jacquemin*
Most Read Articles *What is the Key for Accurate Absorption and Emission Calculations, Energy or Geometry ?*
J. Chem. Theory Comput. (IF=5.313), **14** (2018) 1534–1543 doi.

437. C. A. Guido*, B. Mennucci, G. Sclamani and D. Jacquemin*
Excited State Dipole Moments in Solution: Comparison Between State-Specific and Linear-Response TD-DFT Values
J. Chem. Theory Comput. (IF=5.313), **14** (2018) 1544–1553 doi.

438. M. Ponce-Vargas, B. Stefane, Z. Zaborova, F. Fages, A. D'Aléo, D. Jacquemin* and B. Le Guennic*
Searching for New Borondifluoride-β-diketonate Complexes with Enhanced Absorption/Emission Properties Using Ab Initio *Tools*
Dyes Pigm. (IF=4.018), **155** (2018) 59–67 doi.

439. X. Zhang, D. Jacquemin, Q. Peng*, Z. Shuai* and D. Escudero*
Most Read Articles *A General Approach to Compute Phosphorescent OLED Efficiency*
J. Phys. Chem. C (IF=4.309), **122** (2018) 6340–6347 doi.

440. P. M. Vérité, C. Azarias and D. Jacquemin*
Theoretical Spectroscopy of a NIR-absorbing Benziphthalocyanine Dye
Theor. Chem. Acc. (IF=1.598), **137** (2018) 61 (9p) doi.

441. J. Gurke, S. Budzak, B. M. Schmidt, D. Jacquemin and S. Hecht*
Efficient Light-Induced pK_a-Modulation coupled to Base-Catalyzed Photochromism
Angew. Chem. Int. Ed. (IF=12.257), **57** (2018) 4797–4801 doi.

442. D. Jacquemin and D. Escudero*
2018 PCCP HOT Articles *Thermal Equilibration Between Excited States or Solvent Effects: Unveiling the Origins of Anomalous Emissions in Heteroleptic Ru(II) Complexes*
Phys. Chem. Chem. Phys. (IF=3.567), **20** (2018) 11559–11563 doi.

443. C. Azarias, M. Ponce-Vargas, I. Navizet, P. Fleurat-Lessard, A. Romieu, B. Le Guennic, J. A. Richard*, and D. Jacquemin*
Rationalisation of the Optical Signatures of nor-*Dihydroxanthene-Hemicyanine Fused Near-Infrared Fluorophores By First Principle Tools*
Phys. Chem. Chem. Phys. (IF=3.567), **20** (2018) 12120–12128 doi.

444. K. G. Leslie, D. Jacquemin, E. J. New* and K. A. Jollife*
Expanding the Breadth of 4-Amino-1,8-Naphthalimide Photophysical Properties Through Substitution of the Naphthalimide Core
Chem. Eur. J. (IF=5.160), **24** (2018) 5569–5573 doi.

445. X. Martin-Benlloch, A. Novodomska, D. Jacquemin, E. Davioud-Charvet* and M. Elhabiri*
Iron(III) Coordination Properties of Ladanein, a Flavone Lead with a Broad-Spectrum Antiviral Activity
New. J. Chem. (IF=3.069), **42** (2018) 8074–8087 doi.

446. I. Duchemin*, C. A. Guido, D. Jacquemin and X. Blase*
The Bethe-Salpeter Formalism with Polarizable Continuum Embedding: Reconciling Linear-Response and State-Specific Features
Chem. Sci. (IF=9.556), **9** (2018) 4430–4443 doi.

447. J. Rio, S. Beeck, G. Rotas, S. Ahles, D. Jacquemin, N. Tagmatarchis*, C. Ewels* and H A. Wegner*
Electronic Communication Between two [10]Cycloparaphenylenes and Bisazafullerene $(C_{59}N)_2$ Induced by Cooperative Complexation
Angew. Chem. Int. Ed. (IF=12.257), **57** (2018) 6930–6934 doi.

448. D. Rota Martir, D. B. Cordes, A. M. Z. Slawin, D. Escudero, D. Jacquemin, S. L. Warriner and E. Zysman-Colman*
Luminescent $[Ru_8Pd_4]^{24+}$ Supramolecular Cage
Chem. Comm. (IF=6.164), **54** (2018) 6016–6019 doi.

449. F. Airibi, A. Panossian, D. Jacquemin, J. P. Vors, S. Pazenok, D. R. Leroux* and M. Elhabiri*
A Physico-chemical Investigation on Fluorine-Enriched Quinolines
New J. Chem. (IF=3.069), **42** (2018) 10036–10047 doi.

450. Z. Hong, E. Garoni, A. Colombo, C. Dragonetti*, D. Marinotto, S. Righetto, D. Roberto, D. Jacquemin*, J. Boixel* and V. Guerchais
para-Substituted-1,3-di(2-pyridyl)benzene Platinum(II) Complexes: Photo-modulation of Luminescence and Second-order Nonlinear Optical Properties
Inorg. Chem. (IF=4.850), **57** (2018) 7051–7063 doi.

451. C. Hierlinger, D. Cordes, A. M. Z. Slawin, A. Colombo, C. Dragonetti*, S. Righetto, D. Roberto, D. Jacquemin*, E. Zysman-Colman* and V. Guerchais*
An Investigation on the Second-Order Nonlinear Optical Response of Cationic Bipyridine or Phenanthroline Iridium(III) Complexes Bearing Cyclometallated 2-Phenylpyridines with a Triphenylamine Substituent
Dalton Trans. (IF=4.052), **47** (2018) 8292–8300 doi.

452. H. G. Ruy, M. F. Mayther, J. Tamayo, C. Azarias, E. M. Espinoza, M. Banasiewicz, L. Lukasiewicz, Y. M. Poronik, A. Jezewski, Y. M. Poronik, J. Clark, J. B. Derr K. H. Ahn*, D. T. Gryko*, D. Jacquemin* and V. I. Vullev*
Bidirectional Solvatofluorochromism of a Pyrrolo[3,2-b]pyrrole-diketopyrrolopyrrole Hybrid
J. Phys. Chem. C (IF=4.309), **122** (2018) 13424–134340 doi.

453. D. Rota Martir, A. Pizzolante, D. Escudero, D. Jacquemin*, S. L. Warriner and E. Zysman-Colman*
Photoinduced Energy and Electron Transfer Between a Photoactive Cage Based on a Thermally Activate Delayed Fluorescence Ligand and Encapsulated Fluorescent Dyes
ACS Appl. Energy Mater. (IF=N/A, 2019 FI=4.473), **1** (2018) 2971–2978 doi.

454. L. Kortekaas, J. Chen, D. Jacquemin,* and W. R. Browne*
Most Read Articles *Proton Stabilized Photochemically Reversible E/Z Isomerization of Spiropyrans*
J. Phys. Chem. B (IF=2.923), **122** (2018) 6423–6430 doi.

455. E. Bremond, M. Savarese, C. Adamo* and D. Jacquemin*
Most Read Articles *Accuracy of TD-DFT Geometries: a Fresh Look*
J. Chem. Theory Comput. (IF=5.313), **14** (2018) 3715–3727 doi.

456. A. Scemama, A. Benali, D. Jacquemin, M. Caffarel and P. F. Loos*
Excitation Energies from Diffusion Monte Carlo Using Selected Configuration Interaction Nodes
J. Chem. Phys. (IF=2.997), **149** (2018) 034108 (8 p) doi.

457. S. Gauthier*, A. Porter, S. Achelle, T. Roisnel, V. Dorcet, A. Barsella, N. Le Poul, P. Guevara Level, D. Jacquemin and F. Robin-Le Guen
Mono- and Diplatinum Polyynediyl Complexes as Potential Push-Pull Chromophores: Synthesis, Characterization, TD-DFT Modeling, Photophysical and NLO properties
Organometallics (IF=4.100), **37** (2018) 2232–2244 doi.

458. C. Azarias, S. Pascal, O. Siri* and D. Jacquemin*
Central Substitution of Azacalixphyrins: a Strategy Towards Acidochromic NIR Dyes
Phys. Chem. Chem. Phys. (IF=3.567), **20** (2018) 20056–20069 doi.

459. P. F. Loos, N. Galland and D. Jacquemin*
Most Read Articles
Theoretical 0-0 Energies with Chemical Accuracy
J. Phys. Chem. Lett. (IF=7.329), **9** (2018) 4646–4651 doi.

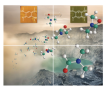
460. J. Massue*, D. Jacquemin* and G. Ulrich*
Molecular Engineering of Excited-State Intramolecular Proton Transfer (ESIPT) Dual and Triple Emitters
Chem. Lett. (IF=1.485), invited review, **47** (2018) 1083–1089 doi.

461. B. Jedrzejewska, A. Skotnicka, A. D. Laurent, M. Pietrzak, D. Jacquemin* and B. Osmialowski*
The Influence of the Nature of the Amino Group in Highly Fluorescent Difluoroborates Exhibiting Intramolecular Charge Transfer
J. Org. Chem. (IF=4.745), **83** (2018) 7779–7788 doi.

462. J. Massue*, A. Felouat, P. M. Vérité, D. Jacquemin*, K. Cyprych, M. Durko, L. Sznitko, J. Mysliwiecc* and G. Ulrich*
Extended Excited-State Intramolecular Proton Transfer (ESIPT) Emitter for Random Lasing Application
Phys. Chem. Chem. Phys. (IF=3.567), **20** (2018) 19958–19963 doi.

463. C. Hierlinger, D. B. Cordes, A. M. Z. Slawin, D. Jacquemin*, V. Guerchais* and E. Zysman-Colman*
Phosphorescent Iridium Complexes Bearing a Nonconjugated Six-Membered Chelating Ring Ancillary Ligand: Tuning Emission Color Towardsx the Blue
Dalton Trans. (IF=4.052), **47** (2018) 10569–10577 doi.

464. P. F. Loos*, A. Scemama, A. Blondel, Y. Garniron, M. Caffarel and D. Jacquemin*
Most Read Articles
A Mountaineering Strategy to Excited States: Highly-Accurate Reference Energies and Benchmarks
J. Chem. Theory Comput. (IF=5.313), **14** (2018) 4360–4379 doi.



465. S. Pascal*, L. Lavaud, C. Azarias, G. Canard, M. Giorgi, D. Jacquemin* and O. Siri*
Controlling the Canonical/Zwitterionic Balance through Intramolecular Proton Transfer: a Strategy for Vapochromism
Mater. Chem. Front. (IF=N/A, 2019 FI=6.788), **2** (2018) 1618–1625 doi.

466. Q. Huaulmé, A. Sutter, S. Fall, D. Jacquemin*, P. Lévêque, P. Retailleau, N. Leclerc* and G. Ulrich*
Versatile Synthesis of α-fused BODIPY Displaying Intense Absorption in the NIR and High Electron Affinity
J. Mater. Chem. C (IF=6.641), **6** (2018) 9925–9931 doi.

467. S. Budzak and D. Jacquemin*
Excited State Intramolecular Proton Transfer in Julolidine Derivatives: an ab initio Study
Phys. Chem. Chem. Phys. (IF=3.567), **20** (2018) 25031–25038 doi.

468. Z. Chen, G. Canard, D. Jacquemin*, C. Bucher, M. Giorgi, and O. Siri*
Heterobimetallic Effect as a new Route to Access Multinuclear Complexes
Inorg. Chem. (IF=4.850), **57** (2018) 12536–12542 doi.

469. L. Lavaud, S. Pascal*, K. Metwally, D. Gasteau, A. Da Silva*, Z. Chen, M. Elhabiri, G. Canard, D. Jacquemin and O. Siri*
Azacalixphyrins as NIR Photoacoustic Contrast Agents
Chem. Comm. (IF=6.164), **54** (2018) 12365–12368 doi.

470. L. Leherte*, A. Petit, D. Jacquemin, D. P. Vercauteren and A. D. Laurent
Investigating Cyclic Peptides Inhibiting CD2-CD58 Interactions through Molecular Dynamics and Molecular Docking Methods
J. Comput. Aided Mol. Des. (IF=3.250), **32** (2018) 1295–1313 doi.

471. K. Gutkowski, C. Azarias, B. Kozankiewicz*, D. Jacquemin* and D. T. Gryko*
Synthesis and Photophysical Properties of N-Arylated Diketopyrrolopyrroles
Eur. J. Org. Chem. (IF=3.029), (2018) 6643–6648 doi.

472. J. Massue*, A. Felouat, M. Curtil, P. M. Vérité, D. Jacquemin* and G. Ulrich*
Solution and Solid-State Excited-State Intramolecular Proton Transfer (ESIPT) Emitters Incorporating Bis-trialkyl-or Triarylsilylethynyl Units
Dyes Pigm. (IF=4.613), **160** (2019) 915–922 doi.

473. F. Barakat, M. Vansteelandt, A. Triastuti, P. Jargeat, D. Jacquemin, J. Graton, K. Mejia, B. Cabanillas, L. Vendier, M. Haddad and N. Fabre*
Bisthiodiketopiperazines with Two Spirocyclic Centers from Lipstick tree derived Endophytic Fungus Botryosphaeria mamane
Phytochemistry (IF=3.044), **158** (2019) 142–148 doi.

474. D. Jacquemin*, M. Khelladi, A. De Nicola and G. Ulrich*
Turning ESIPT-Based Triazine Fluorophores into Dual Emitters: from Theory to Experiment
Dyes Pigm. (IF=4.613), **163** (2019) 475–482 doi.

475. M. Tasior, G. Clermont, M. Blanchard-Desce*, D. Jacquemin* and D. T. Gryko*
Synthesis of Bis(arylethynyl)pyrrolo[3,2-b]pyrroles and an Effect of Intramolecular Charge-transfer on Their Photophysical Behavior
Chem. Eur. J. (IF=4.857), **25** (2019) 598–608 doi.

476. L. Abad Galan, D. B. Bordes, A. M. Z. Slawin, D. Jacquemin*, M. I. Ogden*, M. Massi* and E. Zysman-Colman*
VIP
Analyzing the Relation Between Structure and Aggregation Induced Emission (AIE) Properties of Iridium(III) Complexes through Modification of Non-Chromophoric Ancillary Ligands
Eur. J. Inorg. Chem. (IF=2.529), (2019) 152–163 doi.

477. R. Boyaala, R. Touzani, T. Roisnel, V. Dorcet, E. Caytan, D. Jacquemin*, J. Boixel*, V. Guerchais*, H. Doucet* and J.F. Soulé*
Catalyst-Controlled Regiodivergent C-H Arylation of Fluorinated 2-Arylpyridines and 2-Arylquinolines: Preparation of Luminescent Iridium Complexes
ACS Catal. (IF=12.350), **9** (2019) 1320–1328 doi.

478. P. M. Vérité, C. A. Guido and D. Jacquemin*
2019 PCCP HOT Articles
First-Principle Investigation of the Double ESIPT Process in a Thiophene-Based Dye
Phys. Chem. Chem. Phys. (IF=3.430), **21** (2019) 2307–2317 doi.

479. S. Pascal*, L. Lavaud, C. Azarias, A. Varlot, G. Canard, M. Giorgi, D. Jacquemin* and O. Siri*
Azacalixquinarenes: from Canonical to (Poly-)Zwitterionic Macrocycles through Intramolecular H-Transfer
J. Org. Chem. (IF=4.335), **84** (2019) 1387–1397 doi.

480. M. Munch, M. Curtil, P. M. Vérité, D. Jacquemin*, J. Massue* and G. Ulrich*
Ethynyl-Tolyl Extended 2-(2'-Hydroxyphenyl)benzoxazole Dyes: Solution and Solid-state Excited-State Intramolecular Proton Transfer (ESIPT) Emitters
Eur. J. Org. Chem. (IF=2.889), (2019) 1134–1144 doi.

481. J. P. Cerón-Carrasco* and D. Jacquemin
i-Motif DNA Structures Upon Electric Field Exposure: Completing the Map of Induced Genetic Error
Theor. Chem. Acc. (IF=1.498), **138** (2019) 35 (6 p) doi.

482. P. F. Loos*, M. Boggio-Pasqua, A. Scemama, M. Caffarel and D. Jacquemin
Most Read Articles
Reference Energies for Double Excitations
J. Chem. Theory Comput. (IF=5.011), **15** (2019) 1939–1956 doi.

483. A. Daher, D. Jacquemin, V. Guerchais*, J.F. Soulé* and H. Doucet*
Reactivity of 4-Phenylthiazoles in Ruthenium Catalyzed Direct Arylations
Appl. Organometal. Chem. (IF=3.140), **33** (2019) e4794 (11p) doi.

484. P. F. Loos and D. Jacquemin*
Chemically Accurate 0-0 Energies with not-so-Accurate Excited State Geometries
J. Chem. Theory Comput. (IF=5.011), **15** (2019) 2481–2491 doi.

485. S. Zheng, G. Lingyue, M. J. Hsien Ong, D. Jacquemin, A. Romieu*, J. A. Richard* and R. Srinivasan*
Divergent synthesis of 5',7'-Difluorinated Dihydroxanthene-Hemicyanine Fused Near-Infrared Fluorophores
Org. Biol. Chem. (IF=3.412), **17** (2019) 4291–4300 doi.

486. R. Haldar, A. Mazel, M. Krstic, Q. Zhang, M. Jakoby, I. A. Howard, B. S. Richards, N. Jung, D. Jacquemin, S. Diring* W. Wenzel* F. Odobel* and C. Wöll*
A de novo *Strategy for Predictive Crystal Engineering to Tune Excitonic Coupling*
Nature Commun. (IF=12.121), **10** (2019) 2048 (7 p) doi.

487. G. Bretel, E. Le Grognec, D. Jacquemin, T. Hirose, K. Matsuda and F.X. Felpin*
Fabrication of Robust Spatially-Resolved Photochromic Patterns on Cellulose Papers by Covalent Printing
ACS Appl. Polym. Mater. (IF=N/A, 2019 FI=4.089), **1** (2019) 1240–1250 doi.

488. A. Grabarz, B. Jedrzejewska, A. Skotnicka, N. Arul Murugan, F. Patalas, W. Bartkowiak, D. Jacquemin* and B. Osmialowski*
The Impact of the Heteroatom in Five-Membered Ring on the Photophysical Properties of Difluoroborates
Dyes Pigm. (IF=4.613), **170** (2019) 170481 (12 p) doi.

489. M. Katari, D. Carmichael, D. Jacquemin and G. Frison*
Structure of Electronically Reduced N-Donor Bidentate Ligands and their Heteroleptic Four-coordinate Zinc Complexes: a Survey of DFT Results
Inorg. Chem. (IF=4.825), **58** (2019) 7169–7179 doi.

490. S. Golten, A. Patinec, J. Rocher, K. Akoumany, J. Graton, D. Jacquemin, J. Y. Le Questel, A. Tessier, J. Lebreton, V. Blot, M. Pipelier, J. Le Pendu, B. Linclau* and D. Dubreuil*
3,4-Dideoxy-3,3,4,4-tetrafluoro- and 4-OH Epimeric 3-Deoxy-3,3-difluoro-α-GalCer Analogues: Synthesis and Biological Evaluation on Human iNKT Cells Stimulation
Eur. J. Med. Chem. (IF=5.572), **178** (2019) 195–213 doi.

491. A. Scemama, M. Caffarel, A. Benali, D. Jacquemin and P. F. Loos*
Influence of Pseudopotentials on Excitation Energies From Selected Configuration Interaction and Diffusion Monte Carlo
Res. Chem. (IF=N/A), **1** (2019) 100002 (7 p) doi.

492. F. Legalite, D. Escudero, Y. Pellegrin, E. Blart, D. Jacquemin and F. Odobel*
"Iridium Effect" in Cyclometalated Iridium Complexes for p-Type Dye Sensitized Solar Cells
Dyes Pigm. (IF=4.613), **171** (2019) 107693 (10 p) doi.

493. J. Massue*, T. Pariat, P. M. Vérité, D. Jacquemin*, M. Durko, L. Sznitko, J. Mysliwiec* and G. Ulrich*
Natural Born Laser Dyes: Excited-State Intramolecular Proton Transfer (ESIPT) Emitters and their use in Random Lasing Studies
Nanomaterials (IF=4.324), **9** (2019) 1093 (13 p) doi.

494. P. M. Vérité, S. Hédé and D. Jacquemin*
A Theoretical Elucidation of the Mechanism of Tuneable Fluorescence in a Full-Colour Emissive ESIPT Dye
Phys. Chem. Chem. Phys. (IF=3.430), **21** (2019) 17400–17409 doi.

495. S. Gauthier*, F. Robin-Le Guen, L. Wojcik, N. Le Poul, A. Planchat, Y. Pellegrin*, P. Guevara-Level, N. Szuwarski, M. Boujtita, D. Jacquemin* and F. Odobel*
Synthesis and Properties of Novel Pyranylidene-Based Organic Sensitizers for Dye-Sensitized Solar Cells
Dyes Pigm. (IF=4.613), **171** (2019) 107747 (10p) doi.

496. C. Suellen, R. Garcia Freitas, P. F. Loos and D. Jacquemin*
Most Read Articles
Cross Comparisons Between Experiment, TD-DFT, CC, and ADC for Transition Energies
J. Chem. Theory Comput. (IF=5.011), **15** (2019) 4581–4590 doi.

497. M. Banasiewicz, R. Stezycki, G. D. Kumar, M. Krzeszewski, M. Tasior, B. Koszarna, A. Janiga, O. Vakuliuk, B. Sadowski, D. T. Gryko⋆ and D. Jacquemin⋆
Electronic Communication in Pyrrolo[3,2-b]Pyrroles Possessing Sterically Hindered Aromatic Substituents
Eur. J. Org. Chem. (IF=2.889), (2019) 5247–5253 doi.

498. M. Tasior, B. Koszarna, D. C. Young, B. Bernard, D. Jacquemin⋆, D. Gryko⋆ and D. T. Gryko⋆
Fe^{3+} Catalyzed Synthesis of Pyrrolo[3,2-b]Pyrroles: Formation of New Dyes and Photophysical Studies
Org. Chem. Front. (IF=5.155), **6** (2019) 2939–2948 doi.

499. P. F. Loos and D. Jacquemin⋆
Evaluating 0-0 Energies with Theoretical Tools: a Short Review
ChemPhotoChem (IF=2.838), **3** (2019) 684–696 doi.

500. R. Zalesny⋆, N. Szczotka, A. Grabarz, B. Osmialowski and D. Jacquemin⋆
Design of Two-Photon-Excited Fluorescent Dyes Containing Fluoroborylene Groups
ChemPhotoChem (IF=2.838), **3** (2019) 719–726 doi.

501. S. Pascal, Q. Bellier, S. David, P. A. Bouit, S. H. Chi, N. S. Makarov, B. Le Guennic, S. Chibani, G. Berginc, P. Feneyroux, D. Jacquemin⋆, J. W. Perry, O. Maury⋆ and C. Andraud⋆
Unraveling the Two-Photon Absorption and Excited State Absorption of Aza-BODIPY Dyes for Optical Power Limiting in the SWIR band
J. Phys. Chem. C (IF=4.189), **123** (2019) 23661–23673 doi.

502. P. Guevara-Level, S. Pascal, O. Siri⋆ and D. Jacquemin⋆
First Principles Investigation of the Spectral Properties of Neutral, Zwitterionic, and bis*-Cationic Azaacenes*
Phys. Chem. Chem. Phys. (IF=3.430), **21** (2019) 22910–22918 doi.

503. A. Fihey⋆ and D. Jacquemin⋆
Most Read Articles
Performances of Density Functional Tight-Binding Methods for Describing Ground and Excited State Geometries of Organic Molecules
J. Chem. Theory Comput. (IF=5.011), **15** (2019) 6267–6276 doi.

504. P. L. dos Santos, D. Chen, P. Rajamalli, T. Matulaitis, D. B. Cordes, A. M. Z. Slawin, D. Jacquemin, E. Zysman-Colman⋆ and I. D. W. Samuel⋆
The use of Pyrimidine and Pyrazine Bridges as a Design Strategy to Improve the Performance of Thermally Activated Delayed Fluorescence Organic Light Emitting Diodes
ACS Appl. Mat. Inter. (IF=8.758), **11** (2019) 45171–45179 doi.

505. G. Tang, A. A. Sukhanov, J. Zhao⋆, X. Li, W. Yang, Z. Wang, Liu, Q., V. K. Voronkova⋆, M. Di Donato⋆, D. Escudero⋆ and D. Jacquemin⋆
Red Thermally-Activated Delayed Fluorescence and Intersystem Crossing in Compact Naphthalimide-Phenothiazine Electron Donor/Acceptor Dyads
J. Phys. Chem. C (IF=4.189), **123** (2019) 30171–30186 doi.

506. D. Rota Martir, L. Delforce, D. B. Cordes, A. M. Z. Slawin, S. L. Warriner, D. Jacquemin and E. Zysman-Colman⋆
A Pd_3L_6 Supramolecular Cage Incorporating Photoactive [2.2]Paracyclophane Units
Inorg. Chem. Front. (IF=6.569), **7** (2020) 232–238 doi.

507. A. Chrayteh, C. Ewels⋆ and D. Jacquemin⋆
Dual Fluorescence in Strap ESIPT Systems: A Theoretical Study
Phys. Chem. Chem. Phys. (IF=3.676), **22** (2020) 854–863 doi.

508. L. Lavaud, C. Azarias, G. Canard⋆, S. Pascal, J. Galiana, M. Giorgi, Z. Chen, D. Jacquemin⋆ and O. Siri⋆
Fused Bis-Azacalixphyrin that Reaches NIR-II Absorption
Chem. Comm. (IF=6.222), **56** (2020) 896–899 doi.

509. P. F. Loos* and D. Jacquemin*
Is ADC(3) as Accurate as CC3 for Valence and Rydberg Transition Energies?
J. Phys. Chem. Lett. (IF=6.475), **11** (2020) 974–980 doi.

510. L. Cupellini*, D. Calvani, D. Jacquemin and B. Mennucci*
Charge Transfer from the Carotenoid can Quench Chlorophyll Excitation in Antenna Complexes of Plants
Nature Commun. (IF=14.919), **11** (2020) 662 (8p) doi.

511. R. Duwald, J. Bosson, S. Pascal, S. Grass, F. Zinna, C. Besnard, L. Di Bari, D. Jacquemin* and J. Lacour*
Merging Polyacenes and Cationic Helicenes: from Weak to Intense Chiroptical Properties in the Far Red Region
Chem. Sci. (IF=9.825), **11** (2020) 1165–1169 doi.

512. P. F. Loos*, F. Lippirani*, M. Boggio-Pasqua, A. Scemama and D. Jacquemin*
A Mountaineering Strategy to Excited States: Highly-Accurate Energies and Benchmarks for Medium Size Molecules
J. Chem. Theory Comput. (IF=6.006), **16** (2020) 1711–1741 doi.

513. P. F. Loos*, A. Scemama and D. Jacquemin*
Most Read Articles *The Quest For Highly Accurate Excitation Energies: A Computational Perspective*
J. Phys. Chem. Lett. (IF=6.475), *invited perspective*, **11** (2020) 2374–2383 doi.

514. K. Gutkowski, K. Skonieczny, M. Bugaj, D. Jacquemin* and D. T. Gryko*
First Method for N-Arylation of Diketopyrrolopyrroles with Aryl Triflates
Chem. Asian J. (IF=4.568), **15** (2020) 1369–1375 doi.

515. P. F. Loos*, A. Scemama, I Duchemin, D. Jacquemin* and X. Blase*
Pros and Cons of the Bethe-Salpeter Formalism for Ground-State Energies
J. Phys. Chem. Lett. (IF=6.475), **11** (2020) 3536–3545 doi.

516. S. Gauthier*, F. Robin-Le Guen, L. Wojcik, N. Le Poul, A. Planchat, Y. Pellegrin*, P. Guevara-Level, N. Szuwarski, M. Boujtita, D. Jacquemin* and F. Odobel*
Comparative Studies of New Pyranylidene-Based Sensitizers Bearing Single or Double Anchoring Groups for Dye-Sensitized Solar Cells
Solar Energy (IF=5.742), **205** (2020) 310–319 doi.

517. P. F. Loos*, A. Scemama, M. Boggio-Pasqua and D. Jacquemin*
A Mountaineering Strategy to Excited States: Highly-Accurate Energies and Benchmarks for Exotic Molecules and Radicals
J. Chem. Theory Comput. (IF=6.006), **16** (2020) 3720–3736 doi.

518. D. C. Young, M. Tasior, A. D. Laurent, L. Dobrzycki, M. K. Cyranski, N. Tkachenko*, D. Jacquemin* and D. T. Gryko*
Photostable Orange-Red Emitting Unsymmetrical Diketopyrrolopyrrole-BODIPY Hybrids
J. Mater. Chem. C (IF=7.393), **8** (2020) 7708–7717 doi.

519. L. G. Lukasiewicz, M. Rammo, C. Stark, M. Krzeszewski, D. Jacquemin*, A. Rebane* and D. T. Gryko*
Top Cited *Ground and Excited State Symmetry Breaking and Solvatofluorochromism in Centrosymmetric Pyrrolo[3,2-b]pyrroles Possessing two Nitro Groups*
ChemPhotoChem (IF=3.849), **4** (2020) 508–519 doi.

520. T. Delouche, A. Vacher, E. Caytan, T. Roisnel, B. Le Guennic, D. Jacquemin*, M. Hissler and P. A. Bouit*
Multi-Stage Redox Systems Based on Dicationic P-Containing Polycyclic Aromatic Hydrocarbons
Chem. Eur. J. (IF=5.236), **26** (2020) 8226–8229 doi.

521. B. Osmiamlowski*, E. F. Petrusevich, M. A. Antoniak, I. Grela, M. A. Bin Jassar, M. Nyk, J. M. Luis, B. Jedrzejewska, R. Zalesny and D. Jacquemin*
Controlling Two-Photon Action Cross Section by Changing a Single Heteroatom Position in Fluorescent Dyes
J. Phys. Chem. Lett. (IF=6.475), **11** (2020) 5920–5925 doi

522. L. Favereau*, C. Quinton, C. Poriel, T. Roisnel, D. Jacquemin and J. Crassous
Persistent Organic Room-Temperature Phosphorescence in Cyclohexane-trans-1,2-Bisphthalimide Derivatives: The Dramatic Impact of Heterochiral vs. Homochiral interactions
J. Phys. Chem. Lett. (IF=6.475), **11** (2020) 6426–6434 doi.

523. Z. Chen, K. Lhoussain, C. Bucher, D. Jacquemin*, D. Luneau and O. Siri*
Unconventional Access to Solvatochromic Nickel(II) Dyes Featuring a Coordination-Induced Spin Crossover Behavior
Dyes Pigm. (IF=4.889), **183** (2020) 108645 (7 p) doi.

524. M. Trinel, A. C. Le Lamer*, V. Jullian, D. Jacquemin, J. Graton, V. Cristofoli, E. Crossay, M. Yassine, N. Vergnolle, B. J. Cabanillas, C. Racaud-Sultan* and N. Fabre
Daphnanes Diterpenes from Hura Crepitans L. and Activity Against Human Colorectal Cancer Cells Caco-2
Bioorg. Chem. (IF=5.275), **103** (2020) 104132 (13 p) doi.

525. L. Adair, N. Trinh, P. M. Vérité, D. Jacquemin, K. Jolliffe and E. New*
Synthesis of Aryl-Nitro Functionalised 4-Amino-1,8-Naphthalimides and Their Evaluation as Fluorescent Hypoxia Sensors
Chem. Eur. J. (IF=5.236), **26** (2020) 10064–10071 doi.

526. L. Kortekaas, J. D. Steen, D. R. Duijnstee, D. Jacquemin* and W. R. Browne*
Non-Commutative Switching of Double Spiropyrans
J. Phys. Chem. A (IF=2.781), **124** (2020) 6458–6467 doi.

527. L. Norel*, K. Bernot, F. Gendron, C. A. Gould, T. Roisnel, S. Delbaere, B. Le Guennic, D. Jacquemin, and S. Rigaut.
Coordination-Enhanced Photochromism in Dysprosium Dinuclear Complexes with Photomodulated Single-Molecule Magnet Behavior
Chem. Sq. (IF=NA), **4** (2020) 2 (16 p) doi.

528. X. Blase*, I. Duchemin, D. Jacquemin and P. F. Loos*
Bethe-Salpeter Equation Formalism: From Physics to Chemistry
J. Phys. Chem. Lett. (IF=6.475), *invited perspective*, **11** (2020) 7371–7382 doi.

529. K. Skonieczny, I. Papadopoulos, D. Thiel, K. Gutkowski, P. Haines, P. M. McCosker, A. D. Laurent, P. A. Keller, T. Clark, D. Jacquemin*, D. M. Guldi* and D. T. Gryko*
How to Make Nitroaromatics Glow: Next Generation Large, χ-Shaped, Centrosymmetric Diketopyrrolopyrroles
Angew. Chem. Int. Ed. (IF=15.336), **59** (2020) 16104–16113 doi.

530. T. R. Rusch, A. Schlimm, N. R. Krekiehn, T. Tellkamp, S. Budzak, D. Jacquemin, F. Tuczek, R. Herges and O. M. Magnussen*
Hot Papers *Observation of Collective Photoswitching in Free-Standing TATA-based Azobenzenes on Au(111)*
Angew. Chem. Int. Ed. (IF=15.336), **59** (2020) 17192–17196 doi.

531. M. R. Koli, A. Labiod, S. Chakarborty, M. Kumar, P. Lévêque*, G. Ulrich, N. Leclerc, D. Jacquemin* and S. Mula*
Tuning the Emission Color of Indolo[3,2-b]carbazole based Boron Complexes and their Application in OFET and Bioimaging
ChemPhotoChem (IF=3.849), **4** (2020) 729–741 doi.

532. N. Saleh, A. Bosmani, C. Besnard, T. Bürgi, D. Jacquemin* and J. Lacour*
Simple Access to Novel Chiral Rigid Hemicyanine Fluorophores from Tröger Basesand α-Imino Carbenes
Org. Lett. (IF=6.005), **22** (2020) 7599–7603 doi.

533. P. Liesfeld, Y. Garmshausen, S. Budzak, J. Becker, A. Dallmann, D. Jacquemin* and S. Hecht*
Highly Cooperative Photoswitching in Dihydropyrene Dimers
Angew. Chem. Int. Ed. (IF=15.336), **59** (2020) 19352–19358 doi.

534. H. V. Tran, H. D. Vu, J. Graton, D. Jacquemin, J. Renault and P. Uriac*
Synthesis of Heterocyclic Enamine-Zinc Complexes as Precursors of Stereocontrolled Substitution of Nitrogen α-Position
Tetrahedron Lett. (IF=2.415), **61** (2020) 152405 (4 p) doi.

535. A. Torres Ruiz, M. H. E. Bousquet, S. Pascal*, G. Canard, M. Elhabiri, D. Jacquemin* and O. Siri*
Small Panchromatic and NIR Absorbers from Quinoid Zwitterions and Cations
Org. Lett. (IF=6.005), **22** (2020) 7997–8001 doi.

536. L. Lavaud, C. Azarias, G. Canard, S. Pascal*, D. Jacquemin* and O. Siri*
Pointing Out One Tautomer: Synthesis, Spectroscopic and Theoretical Investigation of a Mixed N-Aryl/Alkyl Substituted Near-Infrared Azacalixphyrin
New. J. Chem. (IF=3.591), **44** (2020) 18130–18137 doi.

537. S. David, D. Chateau, H. J. Chang, L. Karlsson, M. V. Bondar, C. Lopes, B. Le Guennic, D. Jacquemin, G. Berginc, O.Maury*, S. Parola* and C. Andraud*
High Performance Optical Power Limiting Filters at Telecommunication Wavelengths: when aza-BODIPY Dyes Bond to Sol-Gel Materials
J. Phys. Chem. C (IF=4.126), **124** (2020) 24344–24350 doi.

538. A. Chrayteh, C. Ewels* and D. Jacquemin*
TD-DFT and CC2 Insights into the Dual-Emissive Behavior of 2-(2'-Hydroxyphenyl)Oxazoles Core and their Derivatives
Phys. Chem. Chem. Phys. (IF=3.676), **22** (2020) 25066–25074 doi.

539. L. N. Lameijer, S. Budzak, N. A. Simeth, M. J. Hansen, B. L. Feringa, D. Jacquemin* and W. Szymanski*
General Principles for the Design of Visible-Light-Responsive Photoswitches: Tetra-ortho-Chloro-Azobenzenes
Angew. Chem. Int. Ed. (IF=15.336), **59** (2020) 21663–21670 doi.

540. T. Delouche, A. Vacher, T. Roisnel, M. Cordier, J. F. Audibert, B. Le Guennic, F. Miomandre,* D. Jacquemin*, M. Hissler and P. A. Bouit*
Luminescent Molecular Switches Based on Dicationic P-doped Polycyclic Aromatic Hydrocarbons
Mater Adv. (IF=N/A), **1** (2020) 3369–3377 doi.

541. A. Chrayteh, A. Blondel, P. F. Loos and D. Jacquemin*
A Mountaineering Strategy to Excited States: Highly-Accurate Oscillator Strengths and Dipole Moments of Small Molecules
J. Chem. Theory Comput. (IF=6.578), **17** (2021) 416–438 doi.

542. J. F. Longevial, Z. Chen, S. Pascal, D. Jacquemin* and O. Siri*
Stabilization of a 12-Π Electrons Diamino-Benzoquinonediimine Tautomer
Chem. Comm. (IF=6.065), **57** (2021) 548–551 doi.

543. O. D. C. C. De Azevedo,* P. I. P. Elliott*, C. D. Gabbutt, B. M. Heron*, D. Jacquemin*, C. R. Rice and P. A. Scattergood
Quenching of the Phosphorescence of Thermally Reversible Photochromic Naphthopyran Re(I) Complexes Initiated by either Visible or Ultraviolet Radiation
Dalton Trans. (IF=4.569), **50** (2021) 830–834 doi.

544. R. Sarkar, M. Boggio-Pasqua, P. F. Loos* and D. Jacquemin*
Benchmarking TD-DFT and Wave Function Methods for Oscillator Strengths and Excited-State Dipole Moments
J. Chem. Theory Comput. (IF=6.578), **17** (2021) 1117–1132 doi.

545. T. Pariat, M. Munch, M. Durko, J. Mysliwiec, P. Retailleau, P. M. Vérité, D. Jacquemin*, J. Massue* and G. Ulrich*
Impact of Heteroatom Substitution on Dual-State Emissive Rigidified 2-(2'-hydroxyphenyl)benzazole Dyes: Towards Ultra-Bright ESIPT Fluorophores
Chem. Eur. J. (IF=5.020), **27** (2021) 3483–3495 doi.

546. S. David, H. J. Chang, C. Lopez, B. Le Guennic, G. Berginc, E. van Stryland, M. V. Bondar, D. Hagan, D. Jacquemin*, C. Andraud* and O. Maury*
Hot Papers *Benzothiadiazole Substituted aza-BODIPY Dyes: Two-Photon Absorption Enhancement for Improved Optical Limiting Performances at Telecommunication Wavelengths*
Chem. Eur. J. (IF=5.020), **27** (2021) 3517–3525 doi.

547. T. Castaing-Cordier, C. Ladroue, F. Besacier, D. Jacquemin, P. Giraudeau and J. Farjon*
High-field and Benchtop NMR Spectroscopy for the Characterization of New Psychoactive Substances
Forensic Sci. Int. (IF=2.676), **21** (2021) 110718 (8 p) doi.

548. G. D. Kumar, M. Banasiewicz, D. Jacquemin* and D. T. Gryko*
Switch-On Optical Chemosensors for Lithium Ions Based on the Diketopyrrolopyrrole Chromophore
Chem. Asian J. (IF=4.839), **16** (2021) 355–362 doi.

549. M. Véril, A. Scemama, M. Caffarel, F. Lipparini, M. Boggio-Pasqua, D. Jacquemin* and P. F. Loos*
WILEY Top Cited Article 2021-2022 *QUESTDB: a Database of Highly-Accurate Excitation Energies for the Electronic Structure Community*
WIREs Comp. Mol. Sc. (IF=11.500), **11** (2021) e1517 (45 p) doi.

550. T. Pariat, P. M. Vérité, D. Jacquemin*; J. Massue* and G. Ulrich*
2,2-Dipicolylamino Substituted 2-(2'-Hydroxybenzofuranyl) Benzoxazole (HBBO) Derivative : Towards Ratiometric Sensing of Divalent Zinc Cations
Dyes Pigm. (IF=5.122), **190** (2021) 109338 (6 p) doi.

551. J. Bosson*, G. M. Labrador, C. Besnard, D. Jacquemin* and J. Lacour*
Chiral Near-Infrared Fluorophores by Self-Promoted Oxidative Coupling of Cationic Helicenes with Amines/Enamines
Angew. Chem. Int. Ed. (IF=16.823), **60** (2021) 8733–8738 doi.

552. A. Kumar Gupta, W. Li, A. Ruseckas, C. Lian, C. L. Carpenter-Warren, D. B. Cordes, A. M. Z. Slawin, D. Jacquemin*, I. D. W. Samuel* and Eli Zysman-Colman*
Thermally Activated Delayed Fluorescence Emitters with Intramolecular Proton Transfer for High Luminance Solution-Processed Organic Light-Emitting Diodes
ACS Appl. Mat. Inter. (IF=10.383), **13** (2021) 15459–15474 doi.

553. R. J. Durand, S. Achelle, D. Robin-Le Guen, E. Caytan, N. Le Poul, A. Barsella, P. Guevara-Level, D. Jacquemin* and S. Gauthier*
Investigation of Second-Order Nonlinear Optical Responses in a Series of V-Shaped Binuclear Platinum (II) Complexes
Dalton Trans. (IF=4.569), **50** (2021) 4623–4633 doi.

554. J. D. Steen, D. R. Duijnstee, A. S. Sardjan, J. Martinelli, L. Kortekaas, D. Jacquemin* and W. R. Browne*
Most Read Articles *Electrochemically Driven Ring Opening and Closing of a Spiropyran*
J. Phys. Chem. A (IF=2.944), **125** (2021) 3355–3361 doi.

555. B. Osmialowski*, E. F. Petrusevich, K. C. Nawrot, B. K. Paszkiewicz, M. Nyk, J. Zielak, B. Jedrzejewska, J. M. Luis, D. Jacquemin* and R. Zalesny*
Tailoring Nonlinear Absorption of Fluorescent Dyes by Substitution at a Boron Center
J. Mater. Chem. C (IF=8.067), **9** (2021) 6225–6233 doi.

556. D. Jacquemin and J. P. Ceron-Carrasco*
Using Theory to Extend the Scope of Azobenzene Drugs in Chemotherapy: Novel Combinations for a Specific Delivery
ChemMedChem (IF=3.540), **16** (2021) 1764–1774 doi.

557. P. F. Loos*, D. A. Matthews F. Lipparini and D. Jacquemin*
How Accurate are EOM-CC4 Vertical Excitation Energies?
J. Chem. Phys. (IF=4.304), **154** (2021) 221103 (6 p) doi.

558. P. F. Loos*, M. Comin, X. Blase* and D. Jacquemin*
Reference Energies for Intramolecular Charge-Transfer Excitations
J. Chem. Theory Comput. (IF=6.578), **17** (2021) 3666–3686 doi.

559. A. M. Ranieri, M. Vezzelli, K. G. Leslie, S. Huang, S. Stagni, D. Jacquemin, H. Jiang, A. Hubbard, L. Rigamonti, E. Watkin, M. I. Odgen*, E. J. New* and M. Massi*
Structure Illumination Microscopy Imaging of Lipid Vesicles in Live Bacteria with Naphthalimide-Appended Organometallic Complexes
Analyst (IF=5.227), **146** (2021) 3818–3822 doi.

560. Y. Yan, A. A. Sukhanov, M. H. E. Bousquet, Q. Guan, J. Zhao*, V. K. Voronkova*, D. Escudero*, Y. Xing*, G. G. Gurzadyan* and D. Jacquemin*
Does Twisted π-Conjugation Framework Always Induce Efficient Intersystem Crossing? A Case Study with Benzo[b]- and [a]phenanthrene-fused BODIPY Derivatives
J. Phys. Chem. B (IF=3.466), **125** (2021) 6280–6295 doi.

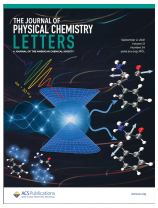
561. Z. Chen, S. Pascal, M. Daurat, L. Lichon, C. Nguyen, A. Godefroy, D. Durand, L. M. A. Ali, N. Bettache, Magali Gary-Bobo*, P. Arnoux, J. F. Longevial, A. D'Aléo, G. Marchand, D. Jacquemin* and O. Siri*
Modified Indulines: From Dyestuffs to in vivo Theranostic Agents
ACS Appl. Mat. Inter. (IF=10.383), **13** (2021) 30337–30349 doi.

562. M. Bondanza, D. Jacquemin and B. Mennucci*
Excited States of Xanthophylls Revised: Towards the Simulation of Biologically Relevant Systems
J. Phys. Chem. Lett. (IF=6.888), **12** (2021) 6604–6612 doi.

563. T. Stoerkler, D. Frath, D. Jacquemin*, J. Massue* and G. Ulrich*
Dual-State Emissive π-Extended Salicylaldehyde Fluorophores: Synthesis, Photophysical Properties and First-Principle Calculations
Eur. J. Org. Chem. (IF=3.261), (2021) 3726–3736 doi.

564. M. Pieczykolan, J. B. Derr*, A. Chrayteh, B. Koszarna, J. A. Clark, O. Vakuliuk, D. Jacquemin*, V. I. Vullev* and D. T. Gryko*
The Synthesis and Photophysical Properties of Weakly-Coupled Diketopyrrolopyrroles
Molecules (IF=4.927), **26** (2021) 4744 (16p) doi.

565. C. A. Guido*, A. Chrayteh, G. Scalmani, B. Mennucci* and D. Jacquemin*
Simple Protocol for Capturing both Linear-Response and State-Specific Effects in Excited-State Calculations with Continuum Solvation Models
J. Chem. Theory Comput. (IF=6.578), **17** (2021) 5155–5164 doi.



566. I. C. D. Merritt, D. Jacquemin and M. Vacher*
Most Read Articles
Attochemistry: Is Controlling Electrons the Future of Photochemistry?
J. Phys. Chem. Lett. (IF=6.888), **12** (2021) 8404–8415 doi.

567. L. Breloy, Rana M., J. P. Malval, V. Brezova, D. Jacquemin*, S. Pascal, O. Siri* and D. L. Versace*
Azacalixphyrins as a Tremendous Alternative for the Free-Radical Photopolymerization under Visible and NIR Irradiation without the Need of Co-Initiators
Chem. Comm. (IF=6.065), **57** (2021) 8973–8976 doi.

568. K. Renault*, A. Chevalier, J. Bignon, D. Jacquemin*, J. A. Richard and A. Romieu*
Unprecedented Coumarin-Pyronin Hybrid Dyes: Synthesis, Fluorescence Properties and Theoretical Calculations
ChemPhotoChem (IF=3.679), **5** (2021) 822–838 doi.

569. I. C. D. Merritt, D. Jacquemin and M. Vacher*
Themed collection
2021 PCCP HOT Articles
Cis → Trans Photoisomerisation of Azobenzene: a Fresh Theoretical Look
Phys. Chem. Chem. Phys. (IF=3.945), **23** (2021) 19155–19165 doi.

570. E. Nikoloudakis, P. Baran Pati, G. Charalambidis, D. S. Budkina, D. Diring, A. Planchat, D. Jacquemin*, E. Vauthey*, A. G. Coutsolelos* and F. Odobel*
Dye-Sensitized PhotoElectrosynthesis Cell (DSPEC) for Benzyl Alcohol Oxidation using Zinc Porphyrin Sensitizer and TEMPO Catalyst
ACS Catal. (IF=13.700), **11** (2021) 12075–12086 doi.

571. M. Winter, M. H. E. Bousquet, D. Jacquemin, I. Duchemin and X. Blase*
Photoluminescent Properties of the Carbon-Dimer Defect in Hexagonal Boron-Nitride: a Many-Body Finite-Size Cluster Approach
Phys. Rev. Mater. (IF=3.980), **5** (2021) 095201 (12p) doi.

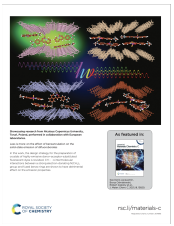
572. Y. Damour, M. Véril, F. Kossoki, M. Caffarel, D. Jacquemin*, A. Scemama* and P. F. Loos*
Accurate Full Configuration Interaction Correlation Energy Estimates for Five- and Six-Membered Rings
J. Chem. Phys. (IF=4.304), **155** (2021) 134104 (14p) doi.

573. P. Vazquez-Dominguez, O. Journaud, N. Vanthuyne, D. Jacquemin*, L. Favereau*, J. Crassous* and A. Ros*
Helical Donor–Acceptor Platinum Complexes Displaying Dual Luminescence and Near-Infrared Circularly Polarized Luminescence
Dalton Trans. (IF=4.569), **50** (2021) 13220–13226 doi.

574. M. E. Graziotto, L. Adair, A. Kaur, P. M. Vérité, S. R. Ball, M. Sunde, D. Jacquemin and E. J. New*
Versatile Naphthalimide Tetrazines for Fluorogenic Bioorthogonal Labelling
RSC Chem. Biol. (IF=N/A), **2** (2021) 1491–1498 doi.

575. J. Massue*, D. Jacquemin* and G. Ulrich*
Boranils: Versatile Multifunctional Organic Fluorophores for Innovative Applications
Organics (IF=N/A), **2** (2021) 365–375 doi.

576. J. Hoffmann, D. Jacquemin, M. Hissler* and A. Staubitz*
BN-Substituted Coronene Diimide Donor-Acceptor-Donor Triads: Photophysical, (Spectro)-Electrochemical Studies and Lewis Behavior
J. Mater. Chem. C (IF=8.067), **9** (2021) 13926–13934 doi.



577. I. Knysh, A. Kozakiewicz, A. Wojtczak, D. Plazuk, G. Baryshnikov, R. Valiev, R. Nasibullin, H. Agren, D. Jacquemin*, B. Osmialowski* and R. Zalesny*
Less is More: On the Effect of Benzannulation on Solid-State Emission of Difluoroborates
J. Mater. Chem. C (IF=8.067), **9** (2021) 15820–15830 doi.

578. P. F. Loos* and D. Jacquemin*
A Mountaineering Strategy to Excited States: Highly-Accurate Energies and Benchmarks for Bicyclic Systems
J. Phys. Chem. A (IF=2.944), **125** (2021) 10174–10188 doi.

579. M. Tasior, P. Kowalczyk, M. Przybyl, M. Czichy, P. Janasik, M. H. E. Bousquet, M. Lapkowski*, M. Rammo, A. Rebane*, D. Jacquemin* and D. T. Gryko*
Going Beyond the Borders: Pyrrolo[3,2-b]pyrroles with Deep Red Emission
Chem. Sci. (IF=9.969), **12** (2021) 15935–15946 doi.

580. T. Pariat, T. Stoerkler, C. Diguet, A. D. Laurent*, D. Jacquemin*, J. Massue* and G. Ulrich*
Dual Solution/Solid-State Emissive Excited-State Intramolecular Proton Transfer (ESIPT) Dyes: a Combined Experimental and Theoretical Investigation
J. Org. Chem. (IF=4.198), **86** (2021) 17606–17619 doi.

581. T. Delouche, G. Taifour, M. Cordier, T. Roisnel, D. Tondelier, P. Manzhi, B. Geffroy, B. Le Guennic, D. Jacquemin*, M. Hissler and P. A. Bouit*
Si-containing Polycyclic Aromatic Hydrocarbons: Synthesis and Opto-electronic Properties
Chem. Comm. (IF=4.9), [4] **58** (2022) 88–91 doi.

582. S. Aiken, G. K. Armitage, O. D. C. C. de Azevedo*, D. L. Crossley, R. Dobson*, C. D. Gabbutt, B. M. Heron*, D. Jacquemin*, C. R. Rice and N. Soltowska*
2,4,6-Tetraryl-2H-benzo[h]chromenes: the Influence of Electronic Communication between Aryl Substituents on their Photochromism
Dyes Pigm. (IF=4.5), **199** (2022) 110036 (24p) doi.

[4] Starting from here, the 2021 IF are used.

583. S. Felder, M. L. Delcourt, M. H. E. Bousquet, D. Jacquemin*, R. Rodriguez, L. Favereau, J. Crassous*, L. Micouin* and E. Benedetti*
Planar Chiral Analogues of PRODAN Based on a [2.2]Paracyclophane Scaffold: Synthesis and Photophysical Studies
J. Org. Chem. (IF=3.6), **87** (2022) 147–158 doi.

584. K. V. Vygranenko, Y. M. Poronik, M. H. E. Bousquet, O. Vakuliuk, D. Jacquemin* and D. T. Gryko*
Direct Transformation of Coumarins into Orange-Red Emitting Rhodols: Unprecedented Reactivity of the Lactone Carbonyl Group
Chem. Comm. (IF=4.9), **58** (2022) 1542–1545 doi.

585. B. Salgues, R. Sarkar, M. L. Fajri, Y. A. Avalos-Quiros, A. D. Manick, M. Giorgi, N. Vanthuyne, Y. Carissan, C. Videlot-Ackermann, J. Ackermann, G. Canard, J. L. Parrain, B. Le Guennic, D. Jacquemin*, M. Amatore, L. Commeiras, E. Zaborova* and F. Fages*
Synthesis and Electron Accepting Properties of Two Di(benz[f]indenone)-fused Tetraazaanthracene Isomers
J. Org. Chem. (IF=3.6), **87** (2022) 3276–3285 doi.

586. M. Munch, E. Colombain, T. Stoerkler, P. M. Vérité, D. Jacquemin*, J. Massue* and G. Ulrich*
Blue-Emitting 2-(2'-Hydroxyphenyl)Benzazole Fluorophores by Modulation of Excited-State Intramolecular Proton Transfer (ESIPT): Spectroscopic Studies and Theoretical Calculations
J. Phys. Chem. B (IF=3.3), **126** (2022) 2108–2118 doi.

587. H. J. Chang, M. V. Bondar, N. Munera, S. David, O. Maury, G. Berginc, B. Le Guennic, D. Jacquemin, C. Andraud, D. J. Hagan* and E. W. Van Stryland
Femtosecond Spectroscopy and Nonlinear Optical Properties of aza-BODIPY Derivatives in Solution
Chem. Eur. J. (IF=4.3), **28** (2022) e202104072 (8p) doi.

588. J. S. A. Badaro, B. Koszarna, M. H. E. Bousquet, E. T. Ouellette, D. Jacquemin* and D. T. Gryko*
The Kröhnke Synthesis of Benzo[a]indolizines Revisited: Towards Small, Red Light Emitters
Org. Chem. Front. (IF=5.4), **9** (2022) 1861–1874 doi.

589. G. D. Kumar, M. Banasiewicz, A. Wrzosek, R. Kempa, M. H. E. Bousquet, D. Jacquemin*, A. Szewczyk* and D. T. Gryko*
Probing Flux of Mitochondrial Potassium using an Azacrown-Diketopyrrolopyrrole based Highly Sensitive Probe
Chem. Comm. (IF=4.9), **58** (2022) 4500–4503 doi.

590. T. Stoerkler, T. Pariat, A. D. Laurent, D. Jacquemin*, G. Ulrich and J. Massue*
Excited-State Intramolecular Proton Transfer Dyes with Dual-State Emission Properties: Concept, Examples and Applications
Molecules (IF=4.6), **27** (2022) 2443 (17p) doi.

591. R. Sarkar, P. F. Loos, M. Boggio-Pasqua* and D. Jacquemin*
Assessing the Performances of CASPT2 and NEVPT2 for Vertical Excitation Energies
J. Chem. Theory Comput. (IF=5.5), **18** (2022) 2418–2436. doi.

592. F. Ceugniet, Q. Huaulmé, A. Sutter, D. Jacquemin*, N. Leclerc* and G. Ulrich*
Hetero-Substituted αβ-Fused BODIPY
Chem. Eur. J. (IF=4.3), **28** (2022) e202200130 (9p) doi.

593. S. Budzak, J. Jovaisaite, C. Y. Huang, P. Baronas, K. Tulaite, S. Jursenas*, D. Jacquemin* and S. Hecht*
Mechanistic Insights into the Photoisomerization of N,N'-Disubstituted Indigos
Chem. Eur. J. (IF=4.3), **28** (2022) e202200496 (9p) doi.

594. M. Boggio-Pasqua*, D. Jacquemin* and P. F. Loos*
Benchmarking CASPT3 Vertical Excitation Energies
J. Chem. Phys. (IF=4.4), **157** (2022) 014103 (14p) doi.

595. P. F. Loos*, F. Lipparini, D. A. Matthews, A. Blondel and Denis Jacquemin*
A Mountaineering Strategy to Excited States: Revising Reference Values with EOM-CC4
J. Chem. Theory Comput. (IF=5.5), **18** (2022) 4418-4427 doi.

596. E. Monino*, M. Boggio-Pasqua, A. Scemama, D. Jacquemin and P. F. Loos*
Reference Energies for Cyclobutadiene: Automerization and Excited States
J. Phys. Chem. A (IF=2.9), **126** (2022) 4664–4679 doi.

597. T. Delouche, E. Caytan, M. Cordier, T. Roisnel, G. Taupier, Y. Molard, N. Vanthuyne, B. Le Guennic, M. Hissler, D. Jacquemin* and P. A. Bouit*
Straightforward Access to Multifunctional π-Conjugated P-Heterocycles Featuring an Internal Ylidic Bond
Angew. Chem. Int. Ed. (IF=16.6), **61** (2022) e202205548 (9p) doi.

598. K. S. Keremane, Y. Pellegrin, A. Planchat, P. Naik, D. Jacquemin*, F. Odobel* and A. V. Adhikari*
New Carbazole-based Dyads for p-Type DSSCs: Impact of Position of Acceptor Units on Device Performance
J. Phys. Chem. C (IF=3.7), **126** (2022) 12383–12390 doi.

599. M. Durko-Maciag, D. Jacquemin*, G. Ulrich, J. Massue* and J. Mysliwiec*
Color-Tunable Multifunctional Excited-State Intramolecular Proton Transfer Emitter: Stimulated Emission of a Single Molecule
Chem. Eur. J. (IF=4.3), **28** (2022) e202201327 (9p) doi.

600. M. Krzeszewski, S. Modrzycka, M. H. E. Bousquet, D. Jacquemin*, M. Drag* and D. T. Gryko*
Green-Emitting 4,5-Diaminonaphthalimides in Activity-based Probes for the Detection of Thrombin
Org. Lett. (IF=5.2), **24** (2022) 5602–5607 doi.

601. T. Stoerkler, T. Pariat, A. D. Laurent, D. Jacquemin*, G. Ulrich*, and J. Massue*
Sterically Hindered 2-(2'-Hydroxyphenyl)benzoxazole (HBO) Emitters: Synthesis, Spectroscopic Studies, and Theoretical Calculations
Eur. J. Org. Chem. (IF=2?8), (2022) e202200661 (8p) doi.

602. K. S. Keremane, Y. Pellegrin, D. Jacquemin*, F. Odobel* and A. V. Adhikari*
Push-pull Phenoxazine-based Sensitizers for p-Type DSSCs: Effect of Acceptor Units on Photovoltaic Performance
ChemSusChem (IF=8.4), **15** (2022) e202200520 (14p) doi.

603. T. Baron, W. Naim,I. Nikolinakos, B. Andrin, Y. Pellegrin, D. Jacquemin*, S. Haacke*, F. Sauvage* and F Odobel*
Transparent and Colorless Dye-Sensitized Solar Cells Based on Pyrrolopyrrole Cyanine Sensitizers
Angew. Chem. Int. Ed. (IF=16.6), **61** (2022) e202207459 (8p) doi.

604. T. Horackova, M. H. E. Bousquet, A. Morice, U. Triballier, G. Canard, P. Lhotak, D. Jacquemin*, S. Pascal* and O. Siri*
Fully Zwitterionic Diaminobenzoquinonediimines Promoted by Cyanoaromatic N-substituents
Dyes Pigm. (IF=4.5), **206** (2022) 110681 (8p) doi.

605. T. Castaing-Cordier, A. Benavides Restrepo, D. Dubois, V. Ladroue, F. Besacier, A. Buleté, C. Charvoz, A. Goupille, D. Jacquemin, P. Giraudeau and J. Farjon*
Characterization of New Psychoactive Substances by Integrating Benchtop NMR to Multi-technique Databases
Drug Test. Analysis (IF=2.9), **14** (2022) 1629–1638 doi.

606. T. Olla, R. Jabbour, A. Labiod, O. Boyron, S. Méry, B. Heinrich, T. Heiser, D. Jacquemin, P. Lévêque, A. Lesage and N. Leclerc*
How Halogenation Impacts the Polymer Backbone Conformation: Learning from Combination of Solid-state MAS NMR and X-Ray Scattering
Adv. Func. Mater. (IF=19.0), **32** (2022) 202204929 (15p) doi.

607. N. Ledos, T. Sangchai, I. Knysh, M. H. E. Bousquet, P. Manzhi, M. Cordier, D. Tondelier, B. Geffroy, D. Jacquemin*, P. A. Bouit* and M. Hissler*
Tuning the Charge Transfer in λ^5-Phosphinines with Amino-Substituents
Org. Lett. (IF=5.2), **24** (2022) 6869–6873 doi.

608. G. D. Kumar, M. Banasiewicz, A. Wrzosek, O. O'Mari, M. Zochowska, V. I. Vullev*, D. Jacquemin*, A. Szewczyk* and D. T. Gryko*
A Sensitive Diketopyrrolopyrrole-based Zinc Probe Operating via Enhancement of Excited-State Intramolecular Charge Transfer
Org. Biomol. Chem. (IF=3.2), **10** (2022) 7439–7447 doi.

609. K. Ye, L. Cao, D. M. E. van Raamsdonk, Z. Wang, Z. Zhao*, D. Escudero* and D. Jacquemin*
Naphthalimide-Phenothiazine Dyads: Effect of Conformational Flexibility and Matching of the Energy of the Charge-Transfer State and the Localized Triplet Excited State on the Thermally Activated Delayed Fluorescence
Beilstein J. Org. Chem. (IF=2.7), **18** (2022) 1435–1453 doi.

610. I. Knysh*, M. B. Jassar, B. Osmialowski, R. Zalesny* and D. Jacquemin*
In silico *Screening of Two-photon Absorption Properties of a Large set of bis-BF_2-Dyes*
ChemPhotoChem (IF=3.7), **6** (2022) e202200137 (9p) doi.

611. T. Stoerkler, A. D. Laurent, G. Ulrich, D. Jacquemin* and J. Massue*
Influence of Ethynyl Extension on the Dual-State Emission Properties of Pyridinium-Substituted ESIPT Fluorophores
Dyes Pigm. (IF=4.5), **208** (2022) 110872 (8p) doi.

612. I. Knysh, I. Duchemin, X. Blase* and D. Jacquemin*
Modelling Excited State Potential Energy Surfaces with Bethe-Salpeter Equation Formalism: The 4-(Dimethylamino)Benzonitrile Twist
J. Chem. Phys. (IF=4.4), **157** (2022) 194102 (13p) doi.

613. P. Rybczyński, M. H. E. Bousquet, A. Kaczmarek-Kedziera, B. Jedrzejewska, D. Jacquemin* and B. Ośmiałowski*
2022 Chemical Science HOT *Controlling the Fluorescence Quantum Yields of Benzothiazole-Difluoroborates by Optimal Substitution*
Chem. Sci. (IF=8.4), **13** (2022) 13347–13360 doi.

614. Xue Zhang, M. Ivanov, A. Wang, M. H. E. Bousquet, X. Liu, Y. Wan, J. Zhao*, A. Barbon*, D. Escudero*, D. Jacquemin* and M. Fedin*
Confinement of the Triplet States in π-Conjugated BODIPY Dimers Linked with Ethyne or Butadiyne Bridges: A Different View on the Effect of Symmetry
Angew. Chem. Int. Ed. (IF=16.6), **61** (2022) e202210419 (8p) doi.

615. Y. Damour*, R. Quintero-Monsebaiz, M. Caffarel, D. Jacquemin, F. Kossoski, A. Scemama and P. F. Loos*
Ground- and Excited-State Dipole Moments and Oscillator Strengths of Full Configuration Interaction Quality
J. Chem. Theory Comput. (IF=5.5), **19** (2023) 221–234 doi.

616. M. Glodek, E. F. Petrusevich, D. Plazuk, D. Jacquemin* and B. Osmialowski*
Polyaromatic Hydrocarbon Antennas as Tools for Tuning properties of Push-Pull Difluoroborates
Dyes Pigm. (IF=4.5), **212** (2023) 111112 (8p) doi.

617. C. Philippe, J. Melan, A. Barsella, T. Vibes, Y. R. Leroux, F. Robin-Le Guen, L. Lemiègre, D. Jacquemin*, S. Gauthier* and Y. Trolez*
A Comprehensive Study of Tetracyanobutadiene Push-Pull Chromophores Derived from γ-Pyranylidene
Tetrahedron Chem. (IF=NA), **5** (2023) 100036 (9p) doi.

618. T. Stoerkler, P. Retailleau, D. Jacquemin, G.Ulrich and J. Massue*
Hetero-Aryl-Substituted bis-Anils: Aggregation-Induced Emission (AIE) Derivatives with Tunable ESIPT Emission Color and pH Sensitivity
Chem. Eur. J. (IF=4.3), **29** (2023) e202203766 (10p) doi.

619. N. Ledos, D. Tondelier, B. Geffroy, D. Jacquemin*, P. A. Bouit* and M. Hissler*
Reaching the 5% Theoretical Limit of Fluorescent OLEDs with Push-Pull Benzophospholes
J. Mater. Chem. C. (IF=6.4), **11** (2023) 3826–3831 doi.

620. J. F. Longevial, I. Knysh, S. Al Shehim, L. Khrouz, A. Pandurangan, S. Pascal, G. Canard, C. Bucher⋆, D. Jacquemini⋆ and O. Siri⋆
Proton-Coupled Electron Transfer in a Pivaloyl-Substituted Dihydro-Tetraazapentacene
Electrochim. Acta (IF=6.6), **449** (2023) 142224 (15p) doi.

621. I. Knysh, K. Letellier, I. Duchemin, X. Blase⋆ and D. Jacquemin⋆
Themed collection 2023 PCCP HOT Articles
Excited State Potential Energy Surfaces of N-Phenylpyrrole upon Twisting: Reference Values and Comparison Between BSE/GW and TD-DFT
Phys. Chem. Chem. Phys. (IF=3.3), **25** (2023) 8376–8385 doi.

622. I. C. D. Merritt, D. Jacquemin and M. Vacher⋆
Non-adiabatic Coupling in Trajectory Surface Hopping: How Approximations Impact Excited-State Reaction Dynamics
J. Chem. Theory Comput. (IF=5.5), **19** (2023) 1827–1842 doi.

623. I. Knysh, J. D. J. Villalobos-Castro, I. Duchemin, X. Blase⋆ and D. Jacquemin⋆
Exploring Bethe-Salpeter Excited-State Dipoles: The Challenging Case of Increasingly Long Push-Pull Oligomers
J. Phys. Chem. Lett. (IF=5.7), **14** (2023) 3727–3734 doi; Err: 5776–5776 doi.

624. J. P. Ceron-Carrasco⋆, N. Sanchez and D. Jacquemin
Optical Signatures of Cisplatin Assembled with Curcuminoids: Theoretical Simulations to Develop Novel Anticancer Prodrugs
Dyes Pigm. (IF=4.5), **216** (2023) 111312 (9p) doi.

625. E. F. Petrusevich, M. H. E. Bousquet, B. Ośmiałowski, D. Jacquemin⋆, J. M. Luis⋆ and R. Zalesny⋆
Cost-Effective Simulations of Vibrationally-Resolved Absorption Spectra of Fluorophores with Machine-Learning-Based Inhomogeneous Broadening
J. Chem. Theory Comput. (IF=5.5), **19** (2023) 2304–2315 doi.

626. T. Munteanu, V. Mazan, M. Elhabiri, C. Benbouziyane, G. Canard, D. Jacquemin⋆, O. Siri⋆ and S. Pascal⋆
A Strategy to Design Substituted Tetraamino-Phenazines and Ac-cess to a NIR-Absorbing Hexaamino-Phenazinium Dye
Org. Lett. (IF=5.2), **25** (2023) 3886–3891 doi.

627. M. Durko-Maciag, G. Ulrich, D. Jacquemin, J. Mysliwiec⋆ and J. Massue⋆
Solid-State Emitters Presenting a Modular Excited-State Proton Transfer (ESIPT) Process: Recent Advances in Dual-State Emission and Lasing Applications
Phys. Chem. Chem. Phys. (IF=3.3), **25** (2023) 15085–15098 doi.

628. C. Figliola⋆, H. Anton, C. Sutter, P. Didier, D. Jacquemin⋆ and G. Ulrich⋆
Lysosomes Targeting pH Activable Imaging-Guided Photodynamic Agents
ChemBioChem (IF=3.2), **24** (2023) e202300139 (10p) doi.

629. T. Stoerkler, G. Ulrich, A. D. Laurent, D.Jacquemin⋆ and J. Massue⋆
Interplay between Dual-State and Aggregation-Induced Emission with ESIPT Scaffolds Containing Triphenylamine Substituents: Experimental and Theoretical Studies
J. Org. Chem. (IF=3.6), **88** (2023) 9225–9236 doi.

630. J. D. J. Villalobos-Castro, I. Knysh, D. Jacquemin, I. Duchemin and X. Blase⋆
Lagrangian Z-vector Approach to Bethe-Salpeter Analytic Gradients: Assessing Approximations
J. Chem. Phys. (IF=4.4), **159** (2023) 024116 (13p) doi.

631. T. Sangchai, N. Ledos, A. Vacher, M. Cordier, B. Le Guennic, M. Hissler, D. Jacquemin⋆ and P. A. Bouit⋆
Intrinsically Switchable Electroactive Fluorophores Based on λ^5-Phosphinine Dimers
Chem. Eur. J. (IF=4.3), **29** (2023) e202301165 (9p) doi.

632. T. Baron, W. Naim, I. Nikolinakos, B. Andrin, Y. Pellegrin, D. Jacquemin⋆, S. Haacke⋆, F. Sauvage⋆ and F. Odobel⋆
Transparent and Colorless DSSC Featuring Thienyl-Pyrrolopyrrole Cyanine Sensitizers
J. Mater. Chem. A (IF=11.9), **11** (2023) 16767–16775 doi.

633. F. Ceugniet⋆, A. Labiod, D. Jacquemin, B. Heinrich, F. Richard, P. Lévêque⋆, G. Ulrich and N. Leclerc⋆
Non-Fused BODIPY-Based Acceptor Molecules for Organic Photovoltaics
J. Mater. Chem. C (IF=6.4), **11** (2023) 10492–12501 doi.

634. M. H. E. Bousquet⋆, T. V. Papineau, K. Veys, D. E. Escudero and D. Jacquemin⋆
Extensive Analysis of the Parameters Influencing Radiative Rates Obtained Through Vibronic Calculations
J. Chem. Theory Comput. (IF=5.5), **19** (2023) 5525–5547 doi.

635. C. Maret, S. Chebourou, A. De Nicola, T. V. Papineau, M. Vacher, D. Jacquemin⋆ and G. Ulrich⋆
Electron Rich Substituted β-Carboline Derivatives: Synthesis and Photophysical Properties
Dyes Pigm. (IF=4.5), **219** (2023) 111640 (8p) doi.

636. T. Baron⋆, V. Maffeis, C. Bucher, B. Le Guennic, A. Banyasz, D.Jacquemin⋆, G. Berginc⋆, O. Maury⋆ and C. Andraud
Tuning the aza-BODIPYs Properties in the Near-Infrared with Thiophene Donor Substituents for Increasing the Charge Transfer
Chem. Eur. J. (IF=4.3), **29** (2023) e202301357 (10p) doi.

637. X. Zhao, I. C. D. Merritt, R. Lei, Y. Shu, D. Jacquemin, L. Zhang⋆, X. Xu⋆, M. Vacher⋆ and D. G. Truhlar⋆
Nonadiabatic Coupling in Trajectory Surface Hopping: Accurate Time Derivative Couplings by the Curvature-Driven Approximation
J. Chem. Theory Comput. (IF=6.578), **19** (2023) 6577–6588 (2023) doi.

638. C. Elian, B. Mourot, C. Benbouziyane, J. P. Malval, S. Lajnef, F. Peyrot, O. Siri, D. Jacquemin⋆, S. Pascal⋆ and D. L. Versace⋆
Tris-benzo[cd]indole Cyanine Enables the NIR-photosensitized Radical and Thiol-ene Polymerizations at 940 nm
Angew. Chem. Int. Ed. (IF=16.6), **62** (2023) e202305963 (9p) doi.

639. I. Knysh, J. Villalobos-Castro, I. Duchemin, X. Blase⋆ and D. Jacquemin⋆
Excess and Excited-State Dipole Moments of Real-Life Dyes: A Comparison Between Wave-Function, BSE/GW, and TD-DFT Values
Phys. Chem. Chem. Phys. (IF=3.3), **25** (2023) 29993–30004 doi.

640. A. F. Henwood⋆, N. Curtin, S. Estalayo-Adrian, S. J. Aramballi, T. Gudmundsson, J. I. Lovitt, L. C. Sigurvinson, H. L. Dalton, C. S. Hawes, D. Jacquemin, D. F. O'Shea⋆ and T. Gunnlaugsson⋆
Accepted *Time-Resolved Fluorescence Imaging with Colour-Changing, "Turn-On/Turn-On" AIE Nanoparticles*
Chem (IF=23.5), accepted (2023).

641. G. Sanil, M. Krzeszewski, W. Danikiewicz, L. Dobrzycki, I. Knysh, L. Dobrzycki, M. K. Cyrabski⋆, D. Jacquemin⋆ and Daniel T. Gryko⋆
Unprecedented 1,2-Aryl Shift Accompanying Double Alkyne Benzannulation
Angew. Chem. Int. Ed. (IF=16.6), accepted (2023) e202311123 (9p) doi.

642. M. T. do Casal, K. Veys, Manon H. E. Bousquet, D. Escudero⋆ and D. Jacquemin⋆
First-Principles Calculations of Excited-State Decay Rate Constants in Organic Fluorophores
J. Phys. Chem. A (IF=2.9), *invited perspective*, accepted doi.

643. D. Jacquemin⋆, F. Kossoski, F. Gam, M. Boggio-Pasqua⋆ and P. F. Loos⋆
Reference Vertical Excitation Energies for Transition Metal Compounds
J. Chem. Theory Comput. (IF=5.5), accepted. doi.

644. T. Castaing-Cordier, S. Crasnier, D. Dubois, V. Ladroue, A. Bulete, C. Prudhomme, C. Charvoz, F. Besacier, D. Jacquemin, P. Giraudeau⋆ and Jonathan Farjon⋆
Non-Uniform Sampling to Enhance the Performance of Compact NMR for Characterizing New Psychoactive Substances
Magn. Reson. Chem. (IF=2.0), accepted.

645. J. A. Clark, D. Kusy, O. Vakuliuk, M. Krzeszewski, K. J. Kochanowski, B. Koszarna, O. O'Mari, D. Jacquemin⋆, D. T. Gryko⋆ and V. I. Vullev⋆
The Magic of Biaryl Linkages: Their Electronic Coupling through them Defines the Propensity for Excited-State Symmetry Breaking in Quadrupolar Acceptor-Donor-Acceptor Fluorophores
Chem. Sci. (IF=8.4), accepted doi.

646. K. Veys, M. H. E. Bousquet, D. Jacquemin and D. Escudero⋆
Modelling the Fluorescence Quantum Yields of Aromatic Compounds: Benchmarking the Machinery to Compute Intersystem Crossing Rates
J. Chem. Theory Comput. (IF=5.5), accepted.

647. A. Chemin, I. Knysh, D. Ari, M. Cordier, T. Roisnel, B. Le Guennic, M. Hissler, D. Jacquemin⋆ and P. A. Bouit⋆
Phospha-cyanines in their Ideal Polymethine State: Synthesis and Structure-Properties Relationships
J. Phys. Chem. A (IF=2.9), accepted.

B Chapters in books

1. D. Jacquemin⋆, E. A. Perpète, B. Champagne, J. M. André and B. Kirtman
Ab Initio Investigations of Polymethineimine Chains for Nonlinear Optics
in *Recent Research Developments in Physical Chemistry* (IF=NA), Research Signpost, G. Pandalai (Ed.)
Vol. **6** (2002) 145–165.

2. D. Y. Zhang⋆, C. Pouchan, D. Jacquemin and E. A. Perpète
Ab Initio Studies of Electronic First Hyperpolarizability of AB Systems Containing Phosphorus and Silicon Atoms
in *Lecture Series in Computer and Computational Sciences*, T. Simos, G. Maroulis (Ed.)
Adv. Comput. Methods Sci. Eng. (IF=NA), **4A–4B** (2005) 667–673.

3. D. Jacquemin⋆, E. A. Perpète and B. Kirtman
Calculation of Hartree-Fock Energy Derivatives in Polymers
in *Multiscale Modelling of Polymer Properties*, E. A. Perpète and M. Laso (Eds.), Computer-Aided Chemical Engineering Series (IF=NA), vol. 22
Chapter **1** (2006) 3–30 isbn.

4. T. J. Shelton, B. Giner, C. S. Adjiman, A. Galindo, G. Jackson⋆, D. Jacquemin, V. Wathelet and E. A. Perpète
The Derivation of Size Parameters for the SAFT-VR Equation of State from Quantum Mechanical Calculation
in *Multiscale Modelling of Polymer Properties*, E. A. Perpète and M. Laso (Eds.), Computer-Aided Chemical Engineering Series (IF=NA), vol. 22
Chapter **7** (2006) 143–159 isbn.

5. F. Odobel⋆, Y. Pellegrin, F. B. Anne and D. Jacquemin
Molecular Engineering of Efficient Dyes for P-type Semiconductor Sensitization
in *High-Efficiency Solar Cells: Physics, Materials and Devices*, X. Wang and Z. M. Wang (Eds.), Materials Science Series (IF=NA), vol. 190
Chapter **8** (2014) 215–246 doi.

6. D. Jacquemin⋆ and C. Adamo
Computational Molecular Electronic Spectroscopy with TD-DFT
in *Density-Functional Methods for Excited States*, N. Ferré, M. Filatov and M. Huix-Rotllant (Eds.)
Top. Curr. Chem. (IF=4.014), **368** (2016) 347–375 doi.

7. D. E. Escudero⋆, A. D. Laurent⋆ and D. Jacquemin⋆
Time-Dependent Density Functional Theory: A Tool to Explore Excited States
in *Handbook of Computational Chemistry*, J. Leszczynski (Ed.), 35 pp doi.

8. M. Boggio-Pasqua, A. Perrier, A Fihey and D. Jacquemin⋆
Modeling Diarylethenes Excited States with Ab initio Tools: from Model Systems to Large Multimers
in *Photon-Working Switches*, Y. Yokoyama and K. Nakatani (Eds.), Chap. 16 (2017) 321–341 doi.

C Editorials

1. M. E. Casida, H. Chermette and D. Jacquemin
Time-Dependent Density Functional Theory for Molecules and Molecular Solids
Editorial as guest editor of a special issue of J. Mol. Struct. (THEOCHEM)
J. Mol. Struct. (THEOCHEM) (IF=1.216), **914** (2009) 1–2 doi.

2. D. Jacquemin⋆, L. Blancafort⋆ and Y. M. Rhee⋆
Most Accessed
Computational Photochemistry
Editorial as guest editor of a special issue of ChemPhotoChem
ChemPhotoChem (IF=2.838), **3** (2019) 664–665 doi.

3. D. Jacquemin⋆, M. Wainwright⋆, and M. B. Heron⋆
Theory is Back in Dyes & Pigments!
Editorial of the journal promoting theory in this (mainly experimental) journal.
Dyes Pigm. (IF=4.889), **176** (2020) 108236 (1p) doi.

D (Published) Proceedings

1. B. Champagne⋆, D. Jacquemin and J. M. André
Model Calculations of the First Hyperpolarizability per Unit Cell of Finite and Infinite Polymethineimine Chains
in *Nonlinear Optical Properties of Organic Materials VIII*, B. J. Thompson (Ed.)
Proc. SPIE (IF=0.077), **2527** (1995) 71–81 doi.

2. D. Jacquemin⋆, B. Champagne and J. M. André
Asymmetric Unit Cell Polymers with Large First Hyperpolarizabilities
Synth. Met. (IF=1.376), **101** (1999) 490–491 doi.

3. S. Pascal, A. Haefele, C. Monnereau, A. Charaf-Eddin, D. Jacquemin, B. Le Guennic, O. Maury⋆ and C. Andraud⋆
On the Versatility of Electronic Structures in Polymethine Dyes
Proc. SPIE (IF=N/A), **9253** (2014) A (11p) doi.

4. S. David⋆, D. Château, H. C. Chang, D. J. Hagan, E. W. Van Stryland, D. Jacquemin, C. Lopes, G. Berginc, S. Parola, O. Maury and C. Andraud
Aza-BODIPY Dyes for Optical Power Limitation in the SWIR: Molecular Engineering for Optimized Hybrid Materials
Proc. SPIE (IF=N/A), **11277** (2020) 25.

5. J. Bosson,⋆ G. M. Labrador, D. Jacquemin⋆ and J. Lacour⋆
Cationic [6]Helicenes: Tuning (Chir)Optical Properties up to the Near Infra-Red
Materials Today: Proceedings (IF= N/A), **62** (2022) 7751–7753 doi.

E Popularization articles

1. D. Jacquemin⋆
Calcul Analytique du Module de Young des Polymères Stéréoréguliers
Chimie Nouvelle (IF=NA), **83** (2003) 124–124.

2. V. Wathelet, C. Michaux, M. Fontaine, J. M. André, D. Jacquemin and E. A. Perpète⋆
Paramétrisation d'Equations d'Etat sur Base de Descripteurs Moléculaires Estimés par la Mécanique Quantique
Techniques de l'Ingénieur (IF=NA), **AF6** (2008) n°052 (17 p.) link.

3. A. D. Laurent⋆, V. Wathelet, M. Bouhy, D. Jacquemin and E. A. Perpète
Simulation de la Perception des Couleurs de Colorants Organiques
Techniques de l'Ingénieur (IF=NA), **AF6** (2010) n°810 (23 p.) link.

4. J. P. Cerón-Carrasco*, D. Jacquemin, J. Zuniga and A. Requena
   Claves Teóricas de la Mutación Espontánea en el ADN
   An. Quím. (IF=N/A), **108** (2012) 197–204.

5. D. Jacquemin* and C. Daniel*
   Molécules et Lumière : une Histoire d'Electrons
   Actual. Chimique (IF=N/A), **382–383** (2014) 93–99.

F Patents

1. O. Siri, Z. Chen and D. Jacquemin
   Analogues of Porphyrins, their Method of Preparation and Use Thereof
   European Patent, EPO n^o 12306044.4

2. K. Benelhadj, J. Massue, G. Ulrich, R. Ziessel, D. Jacquemin and A. D. Laurent
   Emetteur Dual à Base d'Hydroxybenzazoles Substitués
   European Patent, EP 2977374, WO 2016012457.

3. J. Rull-Barrull, M. d'Halluin, D. Jacquemin, E. Le Grognec and F. X. Felpin
   Méthode d'écriture réversible d'un motif sur un élément cellulosique et produit cellulosique associé
   FR 16/00227

4. F. Odobel, F. Sauvage, D. Jacquemin, Y. Pellegrin, T. Baron, W. Naim
   New Derivatives of Pyrrolopyrrole Cyanines and Uses Thereof
   European Patent, EP 4019522.