

Wallonia Alliance for Research in Energy (WARE)
Thematic group on Solar Photovoltaic Energy

Peer-reviewed international publications 2006-2011

1. The Influence of the Intermolecular Orientation on the Photoinduced Charge Transfer Kinetics in Self-Assembled Aggregates of Donor-Acceptor Arrays.
E.H.A. Beckers, S.C.J. Meskers, A.P.H.J. Schenning, Z. Chen, F. Würthner, P.Marsal, D. Beljonne, J. Cornil, and R.A.J. Janssen.
Journal of the American Chemical Society 128 (2006) 649-657.
2. Pathways for Photoinduced Charge Generation and Recombination at Donor-Acceptor Heterojunctions: The Case of Oligophenylenevinylene-Perylene Bisimide Complexes.
A. Burquel, V. Lemaury, D. Beljonne, R. Lazzaroni, and J. Cornil.
Journal of Physical Chemistry A 110 (2006) 3447-3453.
3. Influence of Copolymer Interface Orientation on the Optical Emission of Polymeric Semiconductor Heterojunctions
P. Sreearunothai, A.C. Morteani, I. Avilov, J. Cornil, D. Beljonne, R.H. Friend, R.T. Phillips, C. Silva, and L.M. Herz.
Physical Review Letters 96 (2006) 117403.
4. Charge Hopping in Organic Semiconductors: Influence of Molecular Parameters on Macroscopic Mobilities in Model One-Dimensional Stacks.
Y. Olivier, V. Lemaury, J.L. Brédas, and J. Cornil.
Journal of Physical Chemistry A 110 (2006) 6356-6364.
5. Pathways for Resonant Energy Transfer in Oligo(phenylenevinylene)-Fullerene Dyads: An Atomistic Model.
T.I. Hukka, T. Hoivonen, E. Hennebicq, J.L. Brédas, R.A.J. Janssen, and D. Beljonne.
Advanced Materials 18 (2006) 1301-1306.
6. Effect of Interfaces on the Alignment of a Discotic Liquid-Crystalline Phthalocyanine.
V. De Cupere, J. Tant, P. Viville, R. Lazzaroni, W. Osikowicz, W.R. Salaneck, and Y.H. Geerts.
Langmuir 22 (2006) 7798-7806.
7. Chromophores in Phenylenevinylene-Based Conjugated Polymers: Role of Conformational Kinks and Chemical Defects
E. Hennebicq, C. Deleener, J.L. Brédas, G.D. Scholes, and D. Beljonne.
Journal of Chemical Physics 125 (2006) 054901
8. Transparent, Plastic, Low-Work-Function Poly(3,4-ethylenedioxythiophene) Electrodes.
L. Lindell, A. Burquel, F.L.E. Jacobsson, V. Lemaury, M. Berggren, R. Lazzaroni, J. Cornil, W.R. Salaneck, and X. Crispin.
Chemistry of Materials 18 (2006) 4246-4252.
9. Charge transport properties of a metal-free phthalocyanine discotic liquid crystal.
C. Deibel, D. Janssen, P. Heremans, V. De Cupere, Y. Geerts, M.L. Benkhedir, G.J. Adriaenssens,
Organic Electronics, 2006, 7, 495-499.
10. Highly sensitive spectroscopic characterization of inorganic and organic heterojunctions for solar cells.
K. Vandewal, L. Goris, K. Haenen, Y. Geerts, J. V. Manca,
Eur. Phys. J.: Applied Physics 2006, 36, 281-283.
11. Optical Bandgaps of π -Conjugated Organic Materials at the Polymer Limit: Experiment and Theory.
J. Gierschner, J. Cornil, and H.J. Egelhaaf.
Advanced Materials 19 (2007) 173-191.
12. CT-CT Annihilation in Rigid Perylene End-Capped Pentaphenylanes.

E. Fron, T.D.M. Bell, A. Van Vooren, G. Schweitzer, J. Cornil, D. Beljonne, P. Toele, J. Jacob, K. Müllen, J. Hofkens, M. van der Auweraer, and F.C. De Schryver.
Journal of the American Chemical Society 129 (2007) 610-619.

13. Solid-state Assemblies and Optical Properties of Conjugated Oligomers Combining Fluorene and Thiophene Units.

M. Surin, P. Sonar, A.C. Grimsdale, K. Müllen, S. De Feyter, S. Habuchi, S. Sarzi, E. Braeken, A. Ver Heyen, M. Van der Auweraer, F.C. De Schryver, M. Cavallini, J.F. Moulin, F. Biscarini, C. Femoni, R. Lazzaroni, and Ph. Leclère.

Journal of Materials Chemistry 17 (2007) 728-735.

14. Supramolecular Assembly of Conjugated Polymers: From Molecular Engineering to Solid-State Properties.
Ph. Leclère, M. Surin, P. Brocorens, M. Cavallini, F. Biscarini, and R. Lazzaroni.
Materials Science and Engineering R 55 (2006) 1-56.

15. Non-conjugated, Phenyl Assisted Coupling in Through Bond Electron Transfer in a Perylenemonoimide-Triphenylamine System.

T.D.M. Bell, A. Stefan, V. Lemaur, S. Bernhardt, K. Müllen, J. Cornil, D. Beljonne, J. Hofkens, M. Van der Auweraer, and F.C. De Schryver.
Photochemical & Photobiological Sciences 6 (2007) 406-415.

16. Charge Transport in Organic Semiconductors.

S. Coropceanu, J. Cornil, D.A. da Silva Filho, Y. Olivier, R. Silbey, and J.L. Brédas
Chemical Reviews 107 (2007) 926-952.

17. Impact of Bridging Units on the Dynamics of Charge Generation and Recombination in Organic Solar Cells.

A. Van Vooren, V. Lemaur, A. Ye, D. Beljonne, and J. Cornil
ChemPhysChem 8 (2007) 1240-1249.

18. Influence of Supramolecular Organization on Energy Transfer Properties in Chiral Oligo(p-phenylene vinylene) Porphyrin Assemblies.

F.J.M. Hoeben, M. Wolffs, J. Zhang, S. De Feyter, P. Leclère, A.P.H.J. Schenning, and E.W. Meijer.
Journal of the American Chemical Society 129 (2007) 9819-9828.

19. Singlet-Singlet Annihilation Leading to a Charge-Transfer Intermediate in Chromophore-End-Capped Pentaphenylenes.

E. Fron, G. Schweitzer, J. Jacob, A. Van Vooren, D. Beljonne, K. Müllen, J. Hofkens, M. Van der Auweraer, F.C. De Schryver.
ChemPhysChem 8 (2007) 1386-1393.

20. Liquid Crystalline Octaalkoxycarbonyl Phthalocyanines: Design, Synthesis, Electronic Structure, Self-aggregation and Mesomorphism.

S. Sergeyev, E. Pouzet, O. Debèver, J. Levin, J. Gierschner, J. Cornil, R. G. Aspe, Y. H. Geerts
J. Mater. Chem. 2007, **17**, 1777-1784.

21. Discotic Liquid Crystals: a New Generation of Organic Semiconductors.

S. Sergeyev, W. Pisula, Y. H. Geerts
Chem. Soc. Rev. 2007, **36**, 1902-1929.

22. Energy Transport along Conjugated Polymer Chains: Through-Space or Through-Bond?

Van Averbeke, D. Beljonne, and E. Hennebicq.
Advanced Functional Materials 18 (2008) 492-498.

23. Does Förster Theory Predict the Rate of Electronic Energy Transfer for a Model Dyad at Low Temperature ?

C. Curutchet, B. Mennucci, G.D. Scholes, and D. Beljonne.
Journal of Physical Chemistry B 112 (2008) 3759-3766.

24. Intrachain versus Interchain Electron Transport in Poly(fluorene-*alt*-benzothiadiazole): A Quantum-Chemical Insight.

A. Van Vooren, J.S. Kim, and J. Cornil.

ChemPhysChem 9 (2008) 989-993.

25. Electronic Structures of Interfacial States Formed at Polymeric Semiconductor Heterojunctions.
Y.S. Huang, S. Westenhoff, I. Avilov, P. Sreearunothai, J.M. Hodgkiss, C. Deleener, R.H. Friend, and D. Beljonne.
Nature Materials 7 (2008) 483-489.
26. On the Singlet-Triplet Splitting of Geminate Electron-Hole Pairs in Organic Semiconductors.
S. Difley, D. Beljonne, and T. Van Voorhis.
Journal of the American Chemical Society 130 (2008) 3420-3427.
27. Optoelectronic and Charge Transport Properties at Organic/Organic Semiconductor Interfaces : Comparison between Polyfluorene-Based Polymer Blend and Copolymer.
J.S. Kim, L. Lu, P. Sreearunothai, A. Seeley, K.H. Yim, A. Petruzzella, C.E. Murphy, D. Beljonne, J. Cornil, and R.H. Friend.
Journal of the American Chemical Society 130 (2008) 13120-13131.
28. An Oligomer Study to Small Band Gap Polymers
B.P. Karsten, L. Viani, J. Gierschner, J. Cornil, and R.A.J. Janssen.
Journal of Physical Chemistry A 112 (2008) 10764-10773.
29. Trap Limited Exciton Transport in Conjugated Polymers
S. Athanasopoulos, E. Hennebicq, D. Beljonne, and A.B. Walker.
Journal of Physical Chemistry C 112 (2008) 11532-11538.
30. Conformational Effects on Excitation Transport along Conjugated Polymer Chains.
B. Van Averbeke and D. Beljonne.
Journal of Physical Chemistry A 113 (2009) 2677-2682.
31. Synthesis, Characterization and Comparative Study of Thiophene-Benzothiadiazole Based Donor-Acceptor-Donor (D-A-D) Materials.
P. Sonar, S.P. Singh, Ph. Leclère, M. Surin, R. Lazzaroni, T.T. Lin, A. Dodabalapur, and A. Sellinger.
Journal of Materials Chemistry 19 (2009) 3228-3237.
32. Charge-Transfer Character of Excitons in Poly[2,7-(9,9-di-n-octylfluorene)_(1-x)-co-4,7-(2,1,3-benzothiadiazole)_(x)]
J.M. Winfield, A. Van Vooren, M.J. Park, D.H. Hwang, J. Cornil, J.S. Kim, and R.H. Friend.
Journal of Chemical Physics 131 (2009) 035104.
33. Electronic Structure of Small Band Gap Oligomers Based on Cyclopentadithiophenes and Acceptor Units.
B.P. Karsten, J.C. Bijleveld, L. Viani, J. Cornil, J. Gierschner, and R.A.J. Janssen.
Journal of Materials Chemistry 19 (2009) 5343-5350.
34. On the Origin of Small Band Gaps in Alternating Thiophene – Thienopyrazine Oligomers.
B.P. Karsten, L. Viani, J. Gierschner, J. Cornil, and R.A.J. Janssen.
Journal of Physical Chemistry A 113 (2009) 10343-10350.
35. Theoretical Characterization of the Structural and Hole Transport Dynamics in Liquid-Crystalline Phthalocyanine Stacks.
Y. Olivier, L. Muccioli, V. Lemaur, Y.H. Geerts, C. Zannoni, and J. Cornil.
Journal of Physical Chemistry B 113 (2009) 14102-14111.
36. Molecular Understanding of Organic Solar Cells: The Challenges.
J.L. Brédas, J.S. Norton, J. Cornil, and V. Coropceanu.
Accounts of Chemical Research 42 (2009) 1691-1699.
37. Electronic Structure and Geminate Pair Energetics at Organic/Organic Interfaces: The Case of Pentacene/C₆₀ Heterojunctions.
S. Verlaak, D. Beljonne, D. Cheyns, C. Rolin, M. Linares, F. Castet, J. Cornil, and P. Heremans.
Advanced Functional Materials 19 (2009) 3809-3814.

38. Thiophene-Benzothiadiazole Co-Oligomers: Synthesis, Optoelectronic Properties, Electrical Characterization and Thin-Film Patterning.
 M. Melucci, L. Favaretto, A. Zanelli, M. Cavallini, A. Bongini, P. Maccagnani, P. Ostoja, G. Derue, R. Lazzaroni, and G. Barbarella.
Advanced Functional Materials **20** (2009) 445-452.
39. Plasmonic absorption enhancement in organic solar cells with thin active layers
 H. Shen, P. Bienstman, B. Maes
Journal of Applied Physics, **106**(7), p.073109 (2009)
40. High-efficiency solar cell embedded in SOI substrate for ULP autonomous Circuits
 Bulteel, O.; Delamare, R.; Flandre, D.;
 2009 IEEE International SOI Conference, 5-8 Oct. 2009, California/USA
41. Mechanical properties of anodic aluminum oxide for microelectromechanical system applications
 Moreno-Hagelsieb, L.; Flandre, D.; Raskin, J. -P.
Journal Of Vacuum Science & Technology B, **27** (1) : 542-546 01-02/2009
42. Miscibility between Differently Shaped Mesogens: Structural and Morphological Study of a Phthalocyanine-Perylene Binary System.
 G. Zucchi, P. Viville, B. Donnio, A. Vlad, S. Melinte, M. Mondeshki, R. Graf, H. W. Spiess, Y. H. Geerts, R. Lazzaroni,
J. Phys. Chem. B, **2009**, **113** (16), 5448-5457
43. Metal-Free Phthalocyanines Bearing Eight Alkylsulfonyl Substituents: Design, Synthesis, Electronic Structure, and Mesomorphism of New Electron-Deficient Mesogens.
 Benoît Tylleman, Gabin Gbabode, Claire Amato, Claudine Buess-Herman, Vincent Lemaur, Jérôme Cornil, Rafael Gomez Aspe, Yves Henri Geerts and Sergey Sergeyev,
Chem. Mater., **2009**, **21** (13), 2789–2797
44. Synthesis of mesogenic phthalocyanine-C60 donor-acceptor dyads designed for molecular heterojunction photovoltaic devices.
 Y.H. Geerts, O. Debever, C. Amato, S. Sergeyev,
Beilstein J. Org. Chem. **2009**, **5**, No. 49
45. Control of the porosity of anatase thin films prepared by EISA: Influence of thickness and heat treatment.
 Catherine Henrist, Jennifer Dewalque, François Mathis, Rudi Cloots.
Microporous and Mesoporous Materials **2009**, **117** (1-2), 292-296.
46. Synthesis of diketopyrrolopyrrole (DPP) derivatives comprising bithiophene moieties.
 Sara Stas, Sergey Sergeyev, Yves Geerts.
Tetrahedron, **2010**, **66**, 1837–1845.
47. Charge-Transfer Excitons in Strongly Coupled Organic Semiconductors
 J.F. Glowe, M. Perrin, D. Beljonne, S.C. Hayes, F. Gardebien, and C. Silva.
Physical Review B **81** (2010) 041201.
48. On the Interface Dipole at the Pentacene-Fullerene Heterojunction: A Theoretical Study.
 M. Linares, D. Beljonne, J. Cornil, K. Lancaster, J.L. Brédas, S. Verlaak, A. Mityashin, P. Heremans, A. Fuchs, C. Lennartz, J. Idé, R. Méreau, P. Aurel, L. Ducasse, and F. Castet.
Journal of Physical Chemistry C **114** (2010) 3215-3224.
49. Synthesis and Characterization of Nanocomposites Based on Functional Regioregular Poly(3-hexylthiophene) and Multiwall Carbon Nanotubes.
 F. Boon, S. Desbief, L. Cutaia, O. Douheret, A. Minoia, B. Ruelle, S. Clément, O. Coulembier, J. Cornil, Ph. Dubois, and R. Lazzaroni.
Macromolecular Rapid Communications **31** (2010) 1427-1434.
50. Synthesis of Soluble Oligothiophenes Bearing Cyano Groups, Their Optical and Electrochemical Properties.
 J.Y. Balandier, F. Quist, C. Amato, S. Bouzakraoui, J. Cornil, S. Sergeyev, and Y. Geerts.

Tetrahedron 66 (2010) 9560-9572.

51. Stereocomplexed materials based on poly(3-hexylthiophene)-b-poly(lactide) block copolymers: synthesis by organic catalysis, thermal properties and microscopic morphology;
Grancharov G., Coulembier O., Surin M., Lazzaroni R., Dubois Ph.,
Macromolecules, 43, 8957-8964 (2010)

52. Regioregular poly(3-hexylthiophene)-poly(epsilon-caprolactone) block copolymers: controlled synthesis, microscopic morphology, and charge transport properties;
Surin M., Coulembier O., Tran K., Dewinter J., Leclerc P., Gerbaux P., Lazzaroni R., Dubois Ph.,
Organic Electronics, 11, 767-774 (2010)

53. Synthesis and supramolecular organization of regioregular polythiophene block oligomers: from molecules to nanostructures;
Clement S., Meyer F., De Winter J., Coulembier O., Vande Velde C.M.L., Zeller M., Gerbaux P., Balandier J.Y., Sergeyev S., Lazzaroni R., Geerts Y., Dubois Ph.,
J. Org. Chem., 75, 1561-1568 (2010)

54. Excitation of multiple dipole surface plasmon resonances in spherical silver nanoparticles
Bjoern Niesen, Barry P. Rand, Pol Van Dorpe, H. Shen, B. Maes, Jan Genoe, Paul Heremans,
Optics Express, 18(18), p.19032-19038 (2010)

55. Angle insensitive enhancement of organic solar cells using metallic gratings
A. Abass, H. Shen, P. Bienstman, B. Maes
Journal of Applied Physics, 109, p.023111 (2011)

56. Electronic Processes at Organic/Organic Interfaces: Insight from Modelling and Implications for Opto-Electronic Devices.
D. Beljonne, J. Cornil, F. Castet, L. Muccioli, C. Zannoni, and J.L. Brédas.
Chemistry of Materials 23 (2011) 591-609.

57. Dimers of Anthrathiophene and Anthradithiophene Derivatives: Synthesis and Characterization.
J.Y. Balandier, F. Quist, S. Stas, B. Tylleman, C. Ragoen, A. Mayence, S. Bouzakraoui, J. Cornil, and Y. Geerts.
Organic Letters 13 (2011) 548-551.

58. Tuning the Electronic Coupling in a Low Bandgap Donor-Acceptor Copolymer via the Placement of Side-Chains.
P.M. Oberhumer, Y.S. Huang, S. Massip, D.T. James, G. Tu, S. Albert-Seifried, D. Beljonne, J. Cornil, J.S. Kim, W.T.S. Huck, N.C. Greenham, J. Hodgkiss, and R.H. Friend.
Journal of Chemical Physics 134 (2011) 114901.

59. Novel regioregular poly(3-hexylthiophene)-based polycationic block copolymers.
Tran Nguyen H., Coulembier O., Gerbaux P., De Winter J., Crispin X., Dubois Ph., Polym. Bull., 66, 51-64 (2011)

60. Flat Fresnel doublets made of PMMA and PC: combining low cost production and very high concentration ratio for CPV
Languy, F., Fleury-Frenette, K., Lenaerts, C., Loicq, J., Regaert, D., Thibert, T., & Habraken, S.
Optics Express, 2011, 19(S3), 280-A294.

61. Anthradithiophene Derivatives Substituted at the 2,8-Positions by Formyl and Triphenylamine Units: Synthesis, Optical, and Electrochemical Properties.
J.Y. Balandier, N. Sebaihi, P. Boudard, V. Lemaur, F. Quist, C. Niebel, S. Stas, B. Tylleman, R. Lazzaroni, J. Cornil, Y.H. Geerts; Eur. J. Org. Chem. 2011, 3131–3136.

62. Silaindacenodithiophene Semiconducting Polymers for Efficient Solar Cells and High-Mobility Ambipolar Transistors.
R. S. Ashraf, Z. Chen, D. S. Leem, H. Bronstein, W. Zhang, B. Schroeder, Y. Geerts, J. Smith, S. Watkins, T.D. Anthopoulos, H. Sirringhaus, J.C. de Mello, M. Heeney, I. McCulloch,

63. Thieno[3,2-b]thiophene-Diketopyrrolopyrrole-Containing Polymers for High-Performance Organic Field-Effect Transistors and Organic Photovoltaic Devices.
Hugo Bronstein, Zhuoying Chen, Raja Shahid Ashraf, Weimin Zhang, Junping Du, James R. Durrant, Pabitra Shakya Tuladhar, Kigook Song, Scott E. Watkins, Yves Geerts, Martijn M. Wienk, Rene A. J. Janssen, Thomas Anthopoulos, Henning Sirringhaus, Martin Heeney, and Iain McCulloch,
J. Am. Chem. Soc. 2011, 133, 3272–3275
64. Doping and photo-induced current in discotic liquid crystals thin films: Long-time and temperature effects
Annalisa Calò, Pablo Stoliar, Massimiliano Cavallini, Yves H. Geerts, Fabio Biscarini,
Organic Electronics 2011, 12, 851–856
65. TiO₂ multilayer thick films (up to 4 μm) with ordered mesoporosity: influence of template on the film mesostructure and use as high efficiency photoelectrode in DSSCs.
Jennifer Dewalque, Rudi Cloots, François Mathis, Olivier Dubreuil, Natacha Krins, Catherine Henrist
J. Mater. Chem., 2011, 21, 7356–7363
66. TiO₂ mesoporous thin films studied by Atmospheric Ellipsometric Porosimetry: A case of contamination. O. Dubreuil, J. Dewalque, G. Chêne, F. Mathis, G. Spronck, D. Strivay, R. Cloots, C. Henrist. *Microporous and Mesoporous Materials* (April 2011) doi:10.1016/j.micromeso.2011.04.013
67. Method of fabricating third generation photovoltaic cells based on Si quantum dots using ion implantation
M. Yedji, J. Demarche, G. Terwagne, R. Delamare, D. Flandre, K. Dimitri, G. Ross
Journal of Applied Physics, accepted.
68. Performance comparison of four kinds of flat non-imaging Fresnel lenses made of PC and PMMA for CPV.
Languy, F., Habraken, S., Submitted to *Optics Letters*.
69. Microstructural evolution of a TiO₂ mesoporous monolayer film under calcination: effect of stabilization and repeated thermal treatments on the film crystallization and surface area. Jennifer Dewalque, Rudi Cloots, Olivier Dubreuil, Natacha Krins, Bénédicte Vertruyen and Catherine Henrist. Submitted to *Microporous and Mesoporous Materials*