Illustration of BibTeX usage

Andriy Zhugayevych
a.zhugayevych@skoltech.ru

January 28, 2015

Important note: must be compiled by pdfLaTeX+BibTeX

- Organic electronics [47, 35, 76].
- Organic photovoltaics [36, 12, 25, 90, 72, 57, 69, 16, 34, 22, 13, 46, 11], commercial devices [27, 5], stability [40, 41, 42].
- General photovoltaics [30, 58, 87], PCE limit [60, 28, 49, 58, 74], improving light collection [44, 39], regularly updated data for PCE records [1], AM1.5G solar spectrum [2] in $\mathrm{W/m^2/nm}$.
- Energy and electron transfer in molecular systems [63, 59, 41, 6, 62, 84, 3, 77].
- Surface hopping [61, 81, 26, 67, 73, 88, 89].
- Organic semiconductors modeling: HOMO/LUMO energies and optical bandgap for solar cells [71, 33, 10, 66], charge transport [4, 32, 18, 15, 75, 65, 80, 70, 85, 53, 52, 51, 91], bulk-heterojunction morphology [37, 48].
- Experiment vs. theory: UV-Vis spectra [43, 24, 38, 91], UPS spectra [45, 19, 31, 50, 82].
- Experimental investigations of organic photovoltaic materials: structure-property relationships [20, 86, 56, 79, 83, 64, 29], rational design [55, 7, 54, 17], processing additives [7, 78, 42, 21].
- Structure and polymorphism of molecular crystals [68, 23, 9, 14, 8].

References

[1] http://www.nrel.gov/ncpv/images/efficiency_chart.jpg, National Center for Photovoltaics at NREL: Research Cell Efficiency Records.

[2] http://rredc.nrel.gov/solar/spectra/am1.5/, Reference Solar Spectral Irradiance: Air Mass 1.5.

[3] A. V. Akimov, A. J. Neukirch, and O. V. Prezhdo. Theoretical Insights into Photoinduced Charge Transfer and Catalysis at Oxide Interfaces. *Chem. Rev.*, 113:4496, 2013.

[4] D. Andrienko. Simulations of morphology and charge transport in supramolecular organic materials. *RSC Smart Materials Series*, accepted, 2014.

[5] K. Baeg, M. Caironi, and Y. Noh. Toward Printed Integrated Circuits based on Unipolar or Ambipolar Polymer Semiconductors. *Adv. Mater.*, 25:4210, 2013.

[6] P. F. Barbara, T. J. Meyer, and M. A. Ratner. Contemporary issues in electron transfer research. *J Phys Chem*, 100:13148, 1996.

[7] P. M. Beaujuge and J. M. J. Frechet. Molecular design and ordering effects in pi-functional materials for transistor and solar cell applications. *J. Am. Chem. Soc.*, 133:20009, 2011.

[8] J. Bernstein. *Polymorphism in Molecular Crystals*. Oxford University Press, 2002.

[9] A. D. Bond. Polymorphism in molecular crystals. *Current Opinion in Solid State and Materials Science*, 13:91, 2009.

[10] N. M. Boyle, C. M. Campbell, and G. R. Hutchison. Computational design and selection of optimal organic photovoltaic materials. *J. Phys. Chem. C*, 115:16200, 2011.

[11] C. Brabec, V. Dyakonov, and U. Scherf. *Organic Photovoltaics: Materials, Device Physics, and Manufacturing Technologies*. Wiley, 2008.

[12] C. Brabec, U. Scherf, and V. Dyakonov. *Organic Photovoltaics: Materials, Device Physics, and Manufacturing Technologies*. Wiley, 2014.

[13] Christoph J. Brabec, Srinivas Gowrisanker, Jonathan J. M. Halls, Darin Laird, Shijun Jia, and Shawn P. Williams. Polymerfullerene bulk-heterojunction solar cells. *Advanced Materials*, 22(34):3839, 2010.

[14] D. Braga, F. Grepioni, L. Maini, and M. Polito. Crystal Polymorphism and Multiple Crystal Forms. *Struct Bond*, 132:25, 2009.

[15] J. L. Bredas, D. Beljonne, V. Coropceanu, and J. Cornil. Charge-transfer and energy-transfer processes in π-conjugated oligomers and polymers: a molecular picture. *Chem. Rev.*, 104:4971, 2004.

[16] Fulvio G. Brunetti, Rajeev Kumar, and Fred Wudl. Organic electronics from perylene to organic photovoltaics: painting a brief history with a broad brush. *J. Mater. Chem.*, 20:2934, 2010.

[17] L. Chen, Z. Hong, G. Li, and Y. Yang. Recent progress in polymer solar cells: manipulation of polymer:fullerene morphology and the formation of efficient inverted polymer solar cells. *Adv. Mater.*, 21:1434, 2009.

[18] V. Coropceanu and J. Cornil. D A da Silva Filho, Y Olivier, R Silbey, J L Bredas, Charge transport in organic semiconductors. *Chem. Rev.*, 107:926, 2007.

[19] V. Coropceanu, N. E. Gruhn, S. Barlow, C. Lambert, J. C. Durivage, T. G. Bill, G. Noll, and S. R. Marder. J-L Bredas, Electronic Couplings in Organic Mixed-Valence Compounds: The Contribution of Photoelectron Spectroscopy. *J. Am. Chem. Soc.*, 126:2727, 2004.

[20] J. E. Coughlin, Z. B. Henson, G. C. Welch, and G. C. Bazan. Design and Synthesis of Molecular Donors for Solution-Processed High-Efficiency Organic Solar Cells. *Acc. Chem. Res.*, 47:257, 2014.

[21] R. J. Davey and S. L. M. Schroeder. J H ter Horst, Nucleation of Organic Crystals - A Molecular Perspective. *Angew Chem Int Ed*, 52:2166, 2013.

[22] Carsten Deibel and Vladimir Dyakonov. Polymerfullerene bulk heterojunction solar cells. *Reports on Progress in Physics*, 73(9):096401, 2010.

[23] G. R. Desiraju. Crystal Engineering: From Molecule to Crystal. *J. Am. Chem. Soc.*, 135:9952, 2013.

[24] Marc Dierksen and Stefan Grimme. The vibronic structure of electronic absorption spectra of large molecules: A time-dependent density functional study on the influence of "exact" hartree-fock exchange. *The Journal of Physical Chemistry A*, 108(46):10225, 2004.

[25] Letian Dou, Jingbi You, Ziruo Hong, Zheng Xu, Gang Li, Robert A. Street, and Yang Yang. 25th anniversary article: A decade of organic/polymeric photovoltaic research. *Advanced Materials*, 25(46):6642, 2013.

[26] K. Drukker. Basics of surface hopping in mixed quantum/classical simulations. *J Comput Phys*, 153:225, 1999.

[27] Russell Gaudiana. Organic photovoltaics: Challenges and opportunities. *Journal of Polymer Science Part B: Polymer Physics*, 50(15):1014, 2012.

[28] Noel C. Giebink, Gary P. Wiederrecht, Michael R. Wasielewski, and Stephen R. Forrest. Thermodynamic efficiency limit of excitonic solar cells. *Phys. Rev. B*, 83:195326, May 2011.

[29] G. Giri, E. Verploegen, S. C. B. Mannsfeld, S. Atahan-Evrenk, D. H. Kim, S. Y. Lee, H. A. Becerril, A. Aspuru-Guzik, M. F. Toney, and Z. Bao. Tuning charge transport in solution-sheared organic semiconductors using lattice strain. *Nature*, 480:504, 2011.

[30] M. A. Green. *Third generation photovoltaics: advanced solar energy conversion*. Birkhauser, 2006.

[31] O. L. Griffith, N. E. Gruhn, J. E. Anthony, B. Purushothaman, and D. L. Lichtenberger. Electron transfer parameters of triisopropylsilylethynyl-substituted oligoacenes. *J. Phys. Chem. C*, 112:20518, 2008.

[32] F. C. Grozema and L. D. A. Siebbeles. Mechanism of charge transport in self-organizing organic materials. *Int. Rev. Phys. Chem.*, 27:87, 2008.

[33] Johannes Hachmann, Roberto Olivares-Amaya, Sule Atahan-Evrenk, Carlos Amador-Bedolla, Roel S. Sanchez-Carrera, Aryeh Gold-Parker, Leslie Vogt, Anna M. Brockway, and Alan Aspuru-Guzik. The harvard clean energy project: Large-scale computational screening and design of organic photovoltaics on the world community grid. *The Journal of Physical Chemistry Letters*, 2(17):2241, 2011.

[34] Alexander W. Hains, Ziqi Liang, Michael A. Woodhouse, and Brian A. Gregg. Molecular semiconductors in organic photovoltaic cells. *Chemical Reviews*, 110(11):6689, 2010.

[35] Alan J. Heeger. Semiconducting polymers: the third generation. *Chem. Soc. Rev.*, 39:2354, 2010.

[36] Alan J. Heeger. 25th anniversary article: Bulk heterojunction solar cells: Understanding the mechanism of operation. *Advanced Materials*, 26(1):10, 2014.

[37] M. C. Heiber and A. Dhinojwala. Efficient Generation of Model Bulk Heterojunction Morphologies for Organic Photovoltaic Device Modeling. *Phys. Rev. Applied*, 2:014008, 2014.

[38] G. Heimel, M. Daghofer, J. Gierschner, E. J. W. List, A. C. Grimsdale, K. Mullen, D. Beljonne, J. L. Bredas, and E. Zojer. Breakdown of the mirror image symmetry in the optical absorption/emission spectra of oligo(para-phenylene)s. *J. Chem. Phys.*, 122:054501, 2005.

[39] T. Jageler-Hoheisel, F. Selzer, M. Riede, and K. Leo. Direct Electrical Evidence of Plasmonic Near-Field Enhancement in Small Molecule Organic Solar Cells. *J. Phys. Chem. C*, 118:15128, 2014.

[40] Mikkel Jorgensen, Kion Norrman, Suren A. Gevorgyan, Thomas Tromholt, Birgitta Andreasen, and Frederik C. Krebs. Stability of polymer solar cells. *Advanced Materials*, 24(5):580, 2012.

[41] J. Jortner and M. Bixon. *Electron Transfer–From Isolated Molecules to Biomolecules*, volume 106-107 of *Advances in Chemical Physics*. Wiley, 1999.

[42] L. G. Kaake, G. C. Welch, D. Moses, G. C. Bazan, and A. J. Heeger. Influence of processing additives on charge-transfer time scales and sound velocity in organic bulk heterojunction films. *J. Phys. Chem. Lett.*, 3:1253, 2012.

[43] Stoyan Karabunarliev, Martin Baumgarten, Eric R. Bittner, and Klaus Mullen. Rigorous franck–condon absorption and emission spectra of conjugated oligomers from quantum chemistry. *The Journal of Chemical Physics*, 113(24):11372, 2000.

[44] D. U. Karatay, M. Salvador, K. Yao, A. Jen, and D. S. Ginger. Performance limits of plasmon-enhanced organic photovoltaics. *Appl. Phys. Lett.*, 105:033304, 2014.

[45] S. Kera, H. Yamane, and N. Ueno. First-principles measurements of charge mobility in organic semiconductors: Valence hole-vibration coupling in organic ultrathin films. *Prog Surf Sci*, 84:135, 2009.

[46] Bernard Kippelen and Jean-Luc Bredas. Organic photovoltaics. *Energy Environ. Sci.*, 2:251, 2009.

[47] H. Klauk. *Organic Electronics II: More Materials and Applications*. Wiley, 2012.

[48] L. J. A. Koster. Charge carrier mobility in disordered organic blends for photovoltaics. *Phys. Rev. B*, 81:205318, 2010.

[49] L. J. A. Koster, S. E. Shaheen, and J. C. Hummelen. Pathways to a New Effi ciency Regime for Organic Solar Cells. *Adv. Energy Mater.*, 2:1246, 2012.

[50] S. Krause, M. B. Casu, A. Scholl, and E. Umbach. Determination of transport levels of organic semiconductors by UPS and IPS. *New J Phys*, 10:085001, 2008.

[51] J. J. Kwiatkowski, J. M. Frost, and J. Nelson. The Effect of Morphology on Electron Field-Effect Mobility in Disordered C60 Thin Films. *Nano Lett*, 9:1085, 2009.

[52] J. J. Kwiatkowski, J. Nelson, H. Li, J. L. Bredas, W. Wenzel, and C. Lennartz. Simulating charge transport in tris(8-hydroxyquinoline) aluminium (Alq3). *Phys. Chem. Chem. Phys.*, 10:1852, 2008.

[53] J. A. Letizia, J. Rivnay, A. Facchetti, M. A. Ratner, and T. J. Marks. Variable temperature mobility analysis of n-channel, p-channel, and ambipolar organic field-effect transistors. *Adv Funct Mater*, 20:50, 2010.

[54] G. Li, R. Zhu, and Y. Yang. Polymer solar cells. *Nat Photonics*, 6:153, 2012.

[55] F. Liu, Y. Gu, J. W. Jung, W. H. Jo, and T. P. Russell. On the Morphology of Polymer-Based Photovoltaics. *J Polym Sci Part B Polym Phys*, 50:1018, 2012.

[56] J. Liu, Y. Zhang, H. Phan, A. Sharenko, P. Moonsin, B. Walker, and V. Promarak. T-Q Nguyen, Effects of Stereoisomerism on the Crystallization Behavior and Optoelectrical Properties of Conjugated Molecules. *Adv. Mater.*, 25:3645, 2013.

[57] Richard R. Lunt, Timothy P. Osedach, Patrick R. Brown, Jill A. Rowehl, and Vladimir Bulovic. Practical roadmap and limits to nanostructured photovoltaics. *Advanced Materials*, 23(48):5712, 2011.

[58] T. Markvart and L. Castaner. *Solar cells: materials, manufacture and operation*. Elsevier, 2005.

[59] V. May and O. Kuhn. *Charge and energy transfer dynamics in molecular systems*. Wiley, 2004.

[60] P. K. Nayak and D. Cahen. Updated Assessment of Possibilities and Limits for Solar Cells. *Adv. Mater.*, 26:1622, 2014.

[61] T. Nelson, S. Fernandez-Alberti, A. E. Roitberg, and S. Tretiak. Nonadiabatic Excited-State Molecular Dynamics: Modeling Photophysics in Organic Conjugated Materials. *Acc. Chem. Res.*, 47:1155, 2014.

[62] M. D. Newton. Quantum chemical probes of electron-transfer kinetics: the nature of donor-acceptor interactions. *Chem. Rev.*, 91:767, 1991.

[63] A. Nitzan. *Chemical dynamics in condensed phases*. Oxford University Press, 2006.

[64] Y. Olivier, D. Niedzialek, V. Lemaur, W. Pisula, K. Mullen, U. Koldemir, J. R. Reynolds, R. Lazzaroni, J. Cornil, and D. Beljonne. High-Mobility Hole and Electron Transport Conjugated Polymers: How Structure Defines Function. *Adv. Mater.*, 26:2119, 2014.

[65] Frank Ortmann, Friedhelm Bechstedt, and Karsten Hannewald. Charge transport in organic crystals: Theory and modelling. *physica status solidi (b)*, 248(3):511, 2011.

[66] L. Pandey, C. Risko, J. E. Norton, and J. L. Bredas. Donor-Acceptor Copolymers of Relevance for Organic Photovoltaics: A Theoretical Investigation of the Impact of Chemical Structure Modifications on the Electronic and Optical Properties. *Macromolecules*, 45:6405, 2012.

[67] F. Plasser and H. Lischka. Semiclassical dynamics simulations of charge transport in stacked π-systems. *J. Chem. Phys.*, 134:034309, 2011.

[68] S. L. Price. Predicting crystal structures of organic compounds. *Chemical Society Reviews*, 43:2098, 2014.

[69] Jean Roncali. Single material solar cells: the next frontier for organic photovoltaics? *Advanced Energy Materials*, 1(2):147, 2011.

[70] V. Ruhle, A. Lukyanov, F. May, M. Schrader, T. Vehoff, J. Kirkpatrick, B. Baumeier, and D. Andrienko. Microscopic simulations of charge transport in disordered organic semiconductors. *J. Chem. Theory Comput.*, 7:3335, 2011.

[71] M. C. Scharber, D. Muhlbacher, M. Koppe, P. Denk, C. Waldauf, A.?J. Heeger, and C. J. Brabec. Design rules for donors in bulk-heterojunction solar cellstowards 10% energy-conversion efficiency. *Advanced Materials*, 18:789, 2006.

[72] Cody W. Schlenker and Mark E. Thompson. The molecular nature of photovoltage losses in organic solar cells. *Chem. Commun.*, 47:3702, 2011.

[73] N. Shenvi, J. E. Subotnik, and W. Yang. Simultaneous-trajectory surface hopping: A parameter-free algorithm for implementing decoherence in nonadiabatic dynamics. *J. Chem. Phys.*, 134:144102, 2011.

[74] W. Shockley and H. J. Queisser. Detailed balance limit of efficiency of p-n junction solar cells. *J. Appl. Phys.*, 32:510, 1961.

[75] Z. Shuai, H. Geng, W. Xu, Y. Liao, and J. Andre. From charge transport parameters to charge mobility in organic semiconductors through multiscale simulation. *Chemical Society Reviews*, 43:2662, 2014.

[76] T.A. Skotheim and J.R. Reynolds. *Handbook of Conducting Polymers*. CRC Press, 2007.

[77] J. E. Subotnik, J. Vura-Weis, A. J. Sodt, and M. A. Ratner. Predicting accurate electronic excitation transfer rates via Marcus theory with Boys or Edmiston-Ruedenberg localized diabatization. *J. Phys. Chem. A*, 114:8665, 2010.

[78] Y. Sun, G. C. Welch, W. L. Leong, C. J. Takacs, G. C. Bazan, and A. J. Heeger. Solution-processed small-molecule solar cells with 6.7% efficiency. *Nat Mater*, 11:44, 2012.

[79] C. J. Takacs, Y. Sun, G. C. Welch, L. A. Perez, X. Liu, W. Wen, G. C. Bazan, and A. J. Heeger. Solar cell efficiency, self-assembly, and dipole-dipole interactions of isomorphic narrow-band-gap molecules. *J. Am. Chem. Soc.*, 134:16597, 2012.

[80] A. Troisi. Charge transport in high mobility molecular semiconductors: classical models and new theories. *Chemical Society Reviews*, 40:2347, 2011.

[81] J. C. Tully. Molecular dynamics with electronic transitions. *J. Chem. Phys.*, 93:1061, 1990.

[82] N. Ueno and S. Kera. Electron spectroscopy of functional organic thin films: Deep insights into valence electronic structure in relation to charge transport property. *Prog Surf Sci*, 83:490, 2008.

[83] T. S. van der Poll, A. Zhugayevych, E. Chertkov, R. C. Bakus II, J. E. Coughlin, G. C. Bazan, and S. Tretiak. Polymorphism of crystalline molecular donors for solution-processed organic photovoltaics. *J. Phys. Chem. Lett.*, 5:2700, 2014.

[84] Troy Van Voorhis, Tim Kowalczyk, Benjamin Kaduk, Lee-Ping Wang, Chiao-Lun Cheng, and Qin Wu. The diabatic picture of electron transfer, reaction barriers, and molecular dynamics. *Annual Review of Physical Chemistry*, 61:149, 2010.

[85] L. Viani, Y. Olivier, and S. Athanasopoulos. D A da Silva Filho, J Hulliger, J L Bredas, J Gierschner, J Cornil, Theoretical characterization of charge transport in one-dimensional collinear arrays of organic conjugated molecules. *ChemPhysChem*, 11:1062, 2010.

[86] G. C. Welch, R. C. Bakus, S. J. Teat, and G. C. Bazan. Impact of regiochemistry and isoelectronic bridgehead substitution on the molecular shape and bulk organization of narrow bandgap chromophores. *J. Am. Chem. Soc.*, 135:2298, 2013.

[87] P. Wuerfel and U. Wuerfel. *Physics of solar cells: from basic principles to advanced concepts.* Wiley, 2009.

[88] D. R. Yarkony. Nonadiabatic Quantum Chemistry - Past, Present, and Future. *Chem. Rev.*, 112:481, 2012.

[89] T. Yonehara, K. Hanasaki, and K. Takatsuka. Fundamental Approaches to Nonadiabaticity: Toward a Chemical Theory beyond the Born-Oppenheimer Paradigm. *Chem. Rev.*, 112:499, 2012.

[90] Huaxing Zhou, Liqiang Yang, and Wei You. Rational design of high performance conjugated polymers for organic solar cells. *Macromolecules*, 45(2):607, 2012.

[91] Andriy Zhugayevych, Olena Postupna, Ronald C. Bakus II, Gregory C. Welch, Guillermo C. Bazan, and Sergei Tretiak. Ab initio study of a molecular crystal for photovoltaics: Light absorption, exciton and charge carrier transport. *The Journal of Physical Chemistry C*, 117(10):4920, 2013.