

CURRICULUM VITAE

VEACESLAV COROPCEANU

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Professional Experience

2020-present	Full Research Professor, The University of Arizona
2008-2019	Principal Research Scientist, Georgia Institute of Technology
2005-2008	Senior Research Scientist, Georgia Institute of Technology
2003-2005	Research Scientist II, Georgia Institute of Technology
2000-2003	Research Associate, The University of Arizona
1999- 2000	Research Visitor, Institute of Physics, Luebeck, Germany (Alexander von Humboldt Fellowship)
1997- 1998	Research Visitor, University of Sussex, Brighton, UK (NATO/ Royal Society Fellowship)
1994- 2003	Associate Professor, Moldova State University
1991-1994	Senior Lecturer, Moldova State University
1986-1991	Senior Research Scientist; Moldova State University
1985-1986	Research Scientist; Moldova State University

Education

Ph.D. in Theoretical and Mathematical Physics, Moldova State University, 1985.

B.S. in Physics, Moldova State University, 1982.

Research Interest: Electronic properties of organic and inorganic systems; magnetic properties, molecular electronics, electron transfer, charge and energy transport; interfacial properties; polaron and vibronic coupling theory.

Teaching Experience: Quantum Mechanics, Thermodynamics, Electrodynamics, Statistical Mechanics, Classical Mechanics, Tensor Calculus, Group Theory, Condensed Matter Physics, Electronic Materials.

Professional Activities: reviewer for the NSF, ARL, Science, Nature Materials, Physical Review Letters, Journal of the American Chemical Society, and others.

University Service: Member of the GT Institute Research Faculty Promotions Committee (2014-2019).

Membership: Materials Research Society; American Chemical Society; American Physical Society.

PhD students advised: A. Fonari (2011-2015 Georgia Tech., currently at Schrödinger, N.Y.), Xue-Peng Zhang (exchange student, 2015-2016), M. Guerrero (1993-1996 State U. Moldova, currently at U. El Bosque, Colombia), F. Paladi (1994-1997 Moldova State U., currently at the State U. Moldova).

Funding

NSF/DMR-1105147 - “High Conductivity Binary Organic Single Crystals for Electronic Applications” period -7/1/2011-12/31/2015, amount - \$197,000.

Solvay Specialty Polymers USA, LLC - “Theoretical Investigation of the Photochemical Degradation Pathways in Polysulfones” period- 1/1/2015-12/31/2016, amount- \$120,000.

King Abdullah University of Science and Technology - “Dynamics of Charge Generation and Charge Recombination Processes in Organic Solar Cells: A Multi-Scale Theoretical Study” period- 02/01/2015-12/31/2016, amount- \$200,000.

Army Research Office/W911NF-13-1-0387 “Theory and Experiment of Cocrystals: Principles, Synthesis and Properties” period- 6/1/2014-12/31/2018, amount - \$510,000.

NSF/DMR-1708147 “Excited-State Dynamics in Organic Charge-Transfer Compounds: An Experimental and Theoretical Study” period -8/1/2017-7/31/2021, amount - \$206,200.

NSF/DMR- 2023497 “Excited-State Dynamics in Organic Charge-Transfer Compounds: An Experimental and Theoretical Study” period -1/5/2020-6/31/2022, amount - \$141,000.

Awards

2018- Visiting Professorship, awarded by the Paris//Seine initiative for excellence in research

1999- Alexander von Humboldt Fellowship

1997- NATO/ Royal Society Fellowship

Invited Talks

“Impact of the charge-transfer states on electronic processes in organic solar cells”, Program in Applied Mathematics, University of Arizona, February 24, 2022.

“Charge-Transfer States at Organic-Organic Interfaces: Impact on Charge Recombination Processes” International Conference on NFA-Based Organic Solar Cells: Materials, Morphology and Fundamentals, nanoGe, February 3-4, 2021.

“Charge-Transfer States at Organic-Organic Interfaces: Impact on Electronic Processes”, Department of Chemistry and Biochemistry, University of Arizona, February 24, 2020.

“Theoretical Description of the Electronic Processes in Organic Electronic Devices”, Tsinghua University, November 1, 2019.

“Role of the Charge-Transfer States in Donor-Acceptor Electronic Devices”, Institute of Chemistry Chinese Academy of Sciences, October 30, 2019.

“Role of Charge-Transfer States in Organic Donor-Acceptor Electronic Devices”, Beijing University of Technology, October 29, 2019.

“Nature and Role of Charge-Transfer States in Organic Solar Cells”. 12th International Symposium on Flexible Organic Electronics (ISFOE19), Thessaloniki, Greece, July 2019.

“Electronic processes in organic light emitting diodes: a theoretical perspective”. Laboratory of Physical Chemistry and Polymers, University of Cergy-Pontoise, June, 2019.

“Role of Charge-Transfer States in Organic Donor-Acceptor Electronic Devices”, Linköping University, June 19, 2019.

“Charge-Transfer States at Organic Interfaces: Understanding the Impact of Polarization, Electronic Coupling and Disorder”, Laboratory for Chemistry of Novel Materials, University of Mons/Materia Nova, July, 2018.

“Charge transport and charge recombination in organic donor-acceptor systems”. Laboratory of Physical Chemistry and Polymers, University of Cergy-Pontoise, June, 2018.

“Charge-Transfer States in Organic Solar Cells: Understanding the Impact of Polarization, Delocalization, and Disorder”, Linköping University, June 19, 2017.

“Charge transport and charge recombination in organic solar cells”, Oak Ridge National Laboratory, April 27, 2017.

“Impact of static and dynamic disorder on charge transfer states in organic solar cells”, MRS Fall Meeting, Boston, MA, December 2016.

“Impact of static and dynamic disorder on charge recombination in organic solar cells”, International CECAM-workshop on Computational Insight into Photo-induced Processes at Interfaces, Bremen, Germany, October 2016.

“Charge-recombination processes in organic solar cells: The impact of charge-transfer states”, SPIE, San Diego, August 2016.

“Role of band states and trap states on the charge transport properties of organic semiconductors”, SPIE, San Diego, August 2016.

“Charge Transport in Organic Semiconductors: A Theoretical Characterization of the Microscopic Parameters”, MRS Fall Meeting, Boston, MA, December 2015.

“Charge Transport in Organic Semiconductors: A Theoretical Characterization of the Microscopic Parameters”, International Conference on Charge Transfer and Transport at the Nanoscale, Santiago de Compostela, Spain, September 2015.

“Impact of the active layer morphology on non-geminate recombination dynamics in organic solar cells”, International Conference on Hybrid and Organic Photovoltaics, Rome, Italy, May 2015.

“The effect of static and dynamic disorder on charge transport in organic molecular semiconductor”, State Key Laboratory of Supramolecular Structure and Materials, Jilin University, China, May 2014.

“The effect of static and dynamic disorder on charge transport in organic molecular semiconductor”, Institute of Chemistry, Chinese Academy of Sciences, China, May 2014.

“The effect of static and dynamic disorder on charge transport in organic molecular semiconductor”, International CECAM-Workshop "Charge transport in organic materials", Bremen, Germany, April 2014.

“Charge transport in organic molecular semiconductors: A theoretical perspective”, The 2nd Workshop on Coherent Energy Transport and Optimization in Photosynthesis, Nanyang Technological University, Singapore, January 2014.

“The impact of trap states on electronic processes in organic solar cells”, Center for Advanced Molecular Photovoltaics Annual Meeting, Stanford University, August 2013.

“Electronic Processes in Organic Solar Cells: The Role of Delocalized and Trap States”, International Symposium on Organic Solar Cells: Theory and Experiment, from Description to Prediction, Santa Fe, NM, May 2013.

“The effect of static and dynamic disorder on charge transport in organic molecular semiconductor”, Robert J. Silbey Memorial Symposium on Theory for Experimentalists, Georgia Tech, December 2012.

“The effect of static and dynamic disorder on charge transport in organic molecular semiconductor”, International Symposium on Fundamental Electronic Processes in Organic Semiconductors and Functional Interfaces, Princeton, NJ, October 2012.

“Key electronic processes in organic solar cells: a theoretical perspective”, APS meeting, Boston, March 2012.

“Charge transport in organic semiconductors: A theoretical perspective”, The 6th Japan-Sweden Workshop on Advanced Spectroscopy of Organic Materials for Electronic Applications, Kagasaki, Japan, November 2011.

“Charge transport in organic molecular semiconductors: Interplay between electronic and electron-phonon interactions”, 9th International Conference on Optical Probes of Conjugated Polymers and Organic Nanostructures, Santa Fe, NM, June 2011.

“Charge transport in organic semiconductors: A theoretical perspective”, International Symposium on Organic Transistors and Functional Interfaces, Les Diablerets, Switzerland, May 2010.

Publications (also Koropchanu)

H-index (citations): Google Scholar- 65 (+22000)

(In bold –(co)corresponding author)

1. Zhang, T.; Wang, F.; Kim, H. B.; Choi, I. W.; Wang, C.; Cho, E.; Konefal, R.; Puttison, Y.; Terado, K.; Kobera, L.; Chen, M.; Yang, M.; Bai, S.; Yang, B.; Suo, J.; Yang, S. C.; Liu, X.; Fu, F.; Yoshida, H.; Chen, W. M.; Brus, J.; Coropceanu, V.; Hagfeldt, A.; Brédas, J. L.; Fahlman, M.; Kim, D. S.; Hu, Z.; Gao, F., Ion-modulated radical doping of spiro-OMeTAD for more efficient and stable perovskite solar cells. *Science* **2022**, 377 (6605), 495-501.
2. He, C.; Chen, Z.; Wang, T.; Shen, Z.; Li, Y.; Zhou, J.; Yu, J.; Fang, H.; Li, Y.; Li, S.; Lu, X.; Ma, W.; Gao, F.; Xie, Z.; Coropceanu, V.; Zhu, H.; Bredas, J. L.; Zuo, L.; Chen, H., Asymmetric electron acceptor enables highly luminescent organic solar cells with certified efficiency over 18%. *Nat. Commun.* **2022**, 13, 2598.
3. Luginbuhl, B.; Raval, P.; Pawlak, T.; Du, Z.; Wang, T.; Kupgan, G.; Schopp, N.; Chae, S.; Yoon, S.; Yi, A.; Jung Kim, H.; Coropceanu, V.; Brédas, J.-L.; Nguyen, T.-Q.; Reddy, G. N. M., Resolving Atomic-Scale Interactions in Nonfullerene Acceptor Organic Solar Cells with Solid-State NMR Spectroscopy, Crystallographic Modelling, and Molecular Dynamics Simulations. *Advanced Materials* **2022**, 34, 2105943.
4. Martinati, M.; Wenseleers, W.; Shi, L.; Pratik, S. M.; Rohringer, P.; Cui, W.; Pichler, T.; Coropceanu, V.; Brédas, J.-L.; Cambre, S., Electronic structure of confined carbyne from joint wavelength-dependent resonant Raman spectroscopy and density functional theory investigations. *Carbon* **2022**, 189, 276-283.
5. Cho, E.; Hong, M.; Yang, Y. S.; Cho, Y. J.; **Coropceanu, V.**; Brédas, J.-L., Energy transfer processes in hyperfluorescent organic light-emitting diodes. *Journal of Materials Chemistry C* **2022**, 10, 4629-4636.
6. Pratik, S. M.; **Coropceanu, V.**; Brédas, J.-L., Purely Organic Emitters for Multiresonant Thermally Activated Delay Fluorescence: Design of Highly Efficient Sulfur and Selenium Derivatives. *ACS Materials Letters* **2022**, 4, 440-447.
7. Liu, Y.; Zheng, Z. L.; Coropceanu, V.; Bredas, J. L.; Ginger, D. S., Lower limits for non-radiative recombination loss in organic donor/acceptor complexes. *Mater. Horizons.* **2022**, 9, 325-333.
8. Chen, X. K.; Qian, D. P.; Wang, Y. M.; Kirchartz, T.; Tress, W.; Yao, H. F.; Yuan, J.; Hulsbeck, M.; Zhang, M. J.; Zou, Y. P.; Sun, Y. M.; Li, Y. F.; Hou, J. H.; Inganas, O.; **Coropceanu, V.**; Bredas, J. L.; Gao, F., A unified description of non-radiative voltage losses in organic solar cells. *Nature Energy* **2021**, 6, 799-806.

9. Cho, E.; **Coropceanu, V.**; Bredas, J. L., Impact of chemical modifications on the luminescence properties of organic neutral radical emitters. *J. Mater. Chem. C* **2021**, *9*, 10794-10801.
10. Selezneva, E.; Vercoouter, A.; Schweicher, G.; Lemaur, V.; Broch, K.; Antidormi, A.; Takimiya, K.; Coropceanu, V.; Bredas, J. L.; Melis, C.; Cornil, J.; Siringhaus, H., Strong Suppression of Thermal Conductivity in the Presence of Long Terminal Alkyl Chains in Low-Disorder Molecular Semiconductors. *Adv. Mater.* **2021**, *33*, 2008708.
11. Cho, E.; Hong, M. K.; **Coropceanu, V.**; Bredas, J. L., The Role of Intermolecular Interactions on the Performance of Organic Thermally Activated Delayed Fluorescence (TADF) Materials. *Adv. Opt. Mater.* **2021**, *9*, 2002135.
12. Abroshan, H.; Zhang, Y.; Zhang, X.; Fuentes-Hernandez, C.; Barlow, S.; Coropceanu, V.; Marder, S. R.; Kippelen, B.; Brédas, J. L., Thermally Activated Delayed Fluorescence Sensitization for Highly Efficient Blue Fluorescent Emitters. *Advanced Functional Materials* **2020**, *30*, 2005898.
13. Abroshan, H.; **Coropceanu, V.**; Bredas, J. L., Hyperfluorescence-Based Emission in Purely Organic Materials: Suppression of Energy-Loss Mechanisms via Alignment of Triplet Excited States. *Acs. Mater. Lett.* **2020**, *2*, 1412-1418.
14. Cho, E.; **Coropceanu, V.**; Bredas, J. L., Organic Neutral Radical Emitters: Impact of Chemical Substitution and Electronic-State Hybridization on the Luminescence Properties. *J. Am. Chem. Soc.* **2020**, *142*, 17782-17786.
15. Cho, E.; Liu, L.; **Coropceanu, V.**; Bredas, J. L., Impact of secondary donor units on the excited-state properties and thermally activated delayed fluorescence (TADF) efficiency of pentacarbazole-benzonitrile emitters. *J. Chem. Phys.* **2020**, *153*, 144708.
16. Ashokan, A.; Hanson, C.; Corbin, N.; Brédas, J. L.; **Coropceanu, V.**, Electronic, vibrational, and charge-transport properties of benzothienobenzothiophene–TCNQ co-crystals. *Mater. Chem. Front.* **2020**, *4*, 3623-3631.
17. De Sousa, L. E.; Coropceanu, V.; da Silva Filho, D. A.; Sini, G., On the Physical Origins of Charge Separation at Donor-Acceptor Interfaces in Organic Solar Cells: Energy Bending versus Energy Disorder. *Adv. Theor. Simul.* **2020**, *3*, 1900230.
18. Ashokan, A.; Wang, T. H.; **Coropceanu, V.**; Bredas, J. L., Bulk Heterojunction Solar Cells: Insight into Ternary Blends from a Characterization of the Intermolecular Packing and Electronic Properties in the Corresponding Binary Blends. *Adv. Theor. Simul.* **2020**, *3*, 2000049.
19. Abroshan, H.; Cho, E.; **Coropceanu, V.**; Bredas, J. L., Suppression of Concentration Quenching in Ortho-Substituted Thermally Activated Delayed Fluorescence Emitters. *Adv. Theor. Simul.* **2020**, *3*, 1900185.

20. Abroshan, H.; **Coropceanu, V.**; Bredas, J. L., Radiative and Nonradiative Recombinations in Organic Radical Emitters: The Effect of Guest-Host Interactions. *Adv. Funct. Mater.* **2020**, *30*, 2002916.
21. Cho, E.; **Coropceanu, V.**; Bredas, J. L., Electronic Structure of Multicomponent Organic Molecular Materials: Evaluation of Range-Separated Hybrid Functionals. *J. Chem. Theory Comput.* **2020**, *16*, 3712-3719.
22. Zhang, G. C.; Chen, X. K.; Xiao, J. Y.; Chow, P. C. Y.; Ren, M. R.; Kupgan, G.; Jiao, X. C.; Chan, C. C. S.; Du, X. Y.; Xia, R. X.; Chen, Z. M.; Yuan, J.; Zhang, Y. Q.; Zhang, S. F.; Liu, Y. D.; Zou, Y. P.; Yan, H.; Wong, K. S.; Coropceanu, V.; Li, N.; Brabec, C. J.; Bredas, J. L.; Yip, H. L.; Cao, Y., Delocalization of exciton and electron wavefunction in non-fullerene acceptor molecules enables efficient organic solar cells. *Nature Commun.* **2020**, *11*, 13943.
23. Zheng, Z., Tummala, N. R., Wang, T., **Coropceanu, V.**; Brédas, J. L., Charge Transfer States at Organic-Organic Interfaces: Impact of Static and Dynamic Disorders. *Adv. Energy Mater.* **2019**, *9*, 1803926.
24. Dasari, R. R., Wang, X., Wiscons, R. A., Haneef, H. F., Ashokan, A., Zhang, Y. D., Fonari, M. S., Barlow, S., Coropceanu, V., Timofeeva, T. V., Jurchescu, O. D., Bredas, J. L., Matzger, A. J. & Marder, S. R. Charge-Transport Properties of F(6)TNAP-Based Charge-Transfer Cocrystals. *Adv. Funct. Mater.* **2019**, *29*, 1904858.
25. Coropceanu, V.; Chen, X.-K.; Wang, T.; Zheng, Z.; Brédas, J. L. Charge-transfer electronic states in organic solar cells. *Nature Rev. Mater.* **2019**, *4*, 689-707.
26. Thomas, S.; Li, H.; Dasari, R. R.; Evans, A. M.; Castano, I.; Allen, T. G.; Reid, O. G.; Rumbles, G.; Dichtel, W. R.; Gianneschi, N. C.; Marder, S. R.; **Coropceanu, V.**; Brédas, J. L., Design and synthesis of two-dimensional covalent organic frameworks with four-arm cores: prediction of remarkable ambipolar charge-transport properties. *Mater. Horizons* **2019**, *6*, 1868-1876.
27. Guo, H.; Peng, Q.; Chen, X.-K.; Gu, Q.; Dong, S.; Evans, E. W.; Gillett, A. J.; Ai, X.; Zhang, M.; Credgington, D.; Coropceanu, V.; Friend, R. H.; Brédas, J.-L.; Li, F., High stability and luminescence efficiency in donor-acceptor neutral radicals not following the Aufbau principle. *Nature Mater.* **2019**, *18*, 977-984.
28. Wang, T.; Coropceanu, V.; Brédas, J. L., All-Polymer Solar Cells: Impact of the Length of the Branched Alkyl Side Chains on the Polymer Acceptors on the Interchain Packing and Electronic Properties in Amorphous Blends. *Chem. Mater.* **2019**, *31*, 6239-6248.
29. Wiscons, R. A.; Coropceanu, V.; Matzger A. J., Quaternary Charge-Transfer Solid Solutions: Electronic Tunability through Stoichiometry. *Chem. Mater.* **2019**, *31*, 6598-6604.
30. Chen, X. K.; **Coropceanu, V.**; Bredas, J. L., Assessing the nature of the charge-transfer electronic states in organic solar cells. *Nature Commun.* **2018**, *9*, 5295.

31. Qian, D. P.; Zheng, Z. L.; Yao, H. F.; Tress, W.; Hopper, T. R.; Chen, S. L.; Li, S. S.; Liu, J.; Chen, S. S.; Zhang, J. B.; Liu, X. K.; Gao, B. W.; Ouyang, L. Q.; Jin, Y. Z.; Pozina, G.; Buyanova, I. A.; Chen, W. M.; Inganas, O.; **Coropceanu, V.**; Bredas, J. L.; Yan, H.; Hou, J. H.; Zhang, F. L.; Bakulin, A. A.; Gao, F., Design rules for minimizing voltage losses in high-efficiency organic solar cells. *Nature Mater.* **2018**, *17*, 703-709.
32. Xu, B.; Yi, X. P.; Huang, T. Y.; Zheng, Z. L.; Zhang, J. X.; Salehi, A.; Coropceanu, V.; Ho, C. H. Y.; Marder, S. R.; Toney, M. F.; Bredas, J. L.; So, F.; Reynolds, J. R., Donor Conjugated Polymers with Polar Side Chain Groups: The Role of Dielectric Constant and Energetic Disorder on Photovoltaic Performance. *Adv. Funct. Mater.* **2018**, *28*, 1803418.
33. Goud, N. R., Zhang, X., Brédas, J. L., Coropceanu, V., Matzger, A. J. Discovery of Non-Linear Optical Materials by Function-Based Screening of Multi-Component Solids. *Chem* **2018**, *4*, 150-161.
34. Tu, Z. Y.; Yi, Y. P.; **Coropceanu, V.**; Bredas, J. L., Impact of Phonon Dispersion on Nonlocal Electron-Phonon Couplings in Organic Semiconductors: The Naphthalene Crystal as a Case Study. *J. Phys. Chem. C* **2018**, *122*, 44-49.
35. Lo, C. K.; Gautam, B. R.; Selter, P.; Zheng, Z. L.; Oosterhout, S. D.; Constantinou, I.; Knitsch, R.; Wolfe, R. M. W.; Yi, X. P.; Bredas, J. L.; So, F.; Toney, M. F.; Coropceanu, V.; Hansen, M. R.; Gundogdu, K.; Reynolds, J. R., Every Atom Counts: Elucidating the Fundamental Impact of Structural Change in Conjugated Polymers for Organic Photovoltaics. *Chem. Mater.* **2018**, *30*, 2995-3009.
36. Lo, C. K.; Wang, C.-Y.; Oosterhout, S. D.; Zheng, Z.; Yi, X.; Fuentes-Hernandez, C.; So, F.; Coropceanu, V.; Brédas, J. L.; Toney, M. F.; Kippelen, B.; Reynolds, J. R., Langmuir–Blodgett Thin Films of Diketopyrrolopyrrole-Based Amphiphiles. *ACS Appl. Mater. Inter.* **2018**, *10*, 11995-12004.
37. Sini, G.; Schubert, M.; Risko, C.; Roland, S.; Lee, O. P.; Chen, Z.; Richter, T. V.; Dolfen, D.; Coropceanu, V.; Ludwigs, S.; Scherf, U.; Facchetti, A.; Fréchet, J. M. J.; Neher, D., On the Molecular Origin of Charge Separation at the Donor–Acceptor Interface. *Adv. Energy Mater.* **2018**, 1702232.
38. Tummala, N. R., Aziz, S. G., Coropceanu, V., Bredas, J. L. Characterization of the Structural, Mechanical, and Electronic Properties of Fullerene Mixtures: A Molecular Simulations Description. *J. Mater. Chem. C* **2018**, *6*, 3642-3650.
39. Behera, R. K., Nagula, R. G., Matzger, A. J., Bredas, J. L., **Coropceanu, V.** Electronic Properties of 1,5-Diaminonaphthalene:Tetrahalo-1,4-Benzoquinone Donor-Acceptor Cocrystals. *J. Phys. Chem. C* **2017**, *121*, 23633-23641.
40. Coropceanu, V., Bredas, J. L., Mehraeen, S. Impact of the Active Layer Morphology on Bimolecular Recombination Dynamics in Organic Solar Cells. *J. Phys. Chem. C* **2017**, *45*, 24954-24961.

41. Vermeulen, D., Corbin, N., Goetz, K. P., Jurchescu, O. D., **Coropceanu, V.**, McNeil, L. E. Electron-Phonon Coupling in Anthracene-Pyromellitic Dianhydride. *J. Chem. Phys.* **2017**, *146*, 214705.
42. Lamport, Z. A., Li, R., Wang, C., Mitchell, W., Sparrowe, D., Smilgies, D.-M., Day, C., Coropceanu, V., Jurchescu, O. D. Organic Thin Films with Charge-Carrier Mobility Exceeding That of Single Crystals. *J. Mater. Chem. C* **2017**, *5*, 10313-10319 .
43. Samanta, P. K., Kim, D., Coropceanu, V., Bredas, J. L. Up-Conversion Intersystem Crossing Rates in Organic Emitters for Thermally Activated Delayed Fluorescence: Impact of the Nature of Singlet Vs Triplet Excited States. *J. Am. Chem. Soc.* **2017**, *139*, 4042-4051.
44. Ran, N. A., Roland, S., Love, J. A., Savikhin, V., Takacs, C. J., Fu, Y. T., Li, H., Coropceanu, V., Liu, X. F., Bredas, J. L., Bazan, G. C., Toney, M. F., Neher, D., Nguyen, T. Q. Impact of Interfacial Molecular Orientation on Radiative Recombination and Charge Generation Efficiency. *Nature Commun.* **2017**, *8*, 79.
45. Zheng, Z. L., Egger, D. A., Bredas, J. L., Kronik, L., **Coropceanu, V.** Effect of Solid-State Polarization on Charge-Transfer Excitations and Transport Levels at Organic Interfaces from a Screened Range-Separated Hybrid Functional. *J. Phys. Chem. Lett.* **2017**, *8*, 3277-3283.
46. Zheng, Z. L., Tummala, N. R., Fu, Y. T., **Coropceanu, V.**, Bredas, J. L. Charge-Transfer States in Organic Solar Cells: Understanding the Impact of Polarization, Delocalization, and Disorder. *ACS Appl. Mater. Inter.* **2017**, *9*, 18095-18102.
47. Sutton, C., Tummala, N. R., Kemper, T., Aziz, S. G., Sears, J., **Coropceanu, V.**, Bredas, J. L. Understanding the Effects of Electronic Polarization and Delocalization on Charge-Transport Levels in Oligoacene Systems. *J. Chem. Phys.* **2017**, *146*, 224705.
48. Gali, S. M., D'Avino, G., Aurel, P., Han, G., Yi, Y., Papadopoulos, T. A., Coropceanu, V., Brédas, J. L., Hadziioannou, G., Zannoni, C., Muccioli, L. Energetic Fluctuations in Amorphous Semiconducting Polymers: Impact on Charge-Carrier Mobility. *J. Chem. Phys.* **2017**, *147*, 134904.
49. Zheng, Z., Bredas, J. L., **Coropceanu, V.** Description of the Charge Transfer States at the Pentacene/C₆₀ Interface: Combining Range-Separated Hybrid Functionals with the Polarizable Continuum Model. *J. Phys. Chem. Lett.* **2016**, *7*, 2616-2621.
50. Tummala, N. R., Elroby, S. A., Aziz, S. G., Risko, C., **Coropceanu, V.**, Bredas, J. L. Packing and Disorder in Substituted Fullerenes. *J. Phys. Chem. C* **2016**, *120*, 17242-17250.
51. Sweetnam, S., Vandewal, K., Cho, E., Risko, C., Coropceanu, V., Salleo, A., Bredas, J. L., McGehee, M. D. Characterizing the Polymer:Fullerene Intermolecular Interactions. *Chem. Mater.* **2016**, *28*, 1446-1452.

52. Goetz, K. P., Tsutsumi, J. Y., Pookpanratana, S., Chen, J., Corbin, N. S., Behera, R. K., Coropceanu, V., Richter, C. A., Hacker, C. A., Hasegawa, T., Jurchescu, O. D. Polymorphism in the 1:1 Charge-Transfer Complex DBTTF–TCNQ and Its Effects on Optical and Electronic Properties. *Adv. Electron. Mater.* **2016**, 2, 1600203.
53. Giesecking, R. L., Ravva, M. K., Coropceanu, V., Bredas, J. L. Benchmarking Density Functional Theory Approaches for the Description of Symmetry Breaking in Long Polymethine Dyes. *J. Phys. Chem. C* **2016**, 120, 9975-9984.
54. Conboy, G., Spencer, H. J., Angioni, E., Kanibolotsky, A. L., Findlay, N. J., Coles, S. J., Wilson, C., Pitak, M. B., Risko, C., Coropceanu, V., Bredas, J. L., Skabara, P. J. To Bend or Not to Bend - Are Heteroatom Interactions within Conjugated Molecules Effective in Dictating Conformation and Planarity? *Materials Horizons* **2016**, 3, 333-339.
55. Tummala, N. R., Zheng, Z. L., Aziz, S. G., **Coropceanu, V.**, Bredas, J. L. Static and Dynamic Energetic Disorders in the C₆₀, PC₆₁BM, C₇₀, and PC₇₁BM Fullerenes. *J. Phys. Chem. Lett.* **2015**, 6, 3657-3662.
56. Stevens, L. A., Goetz, K. P., Fonari, A., Shu, Y., Williamson, R. M., Bredas, J. L., **Coropceanu, V.**, Jurchescu, O. D., Collis, G. E. Temperature-Mediated Polymorphism in Molecular Crystals: The Impact on Crystal Packing and Charge Transport. *Chem. Mater.* **2015**, 27, 112-118.
57. Fonari, A., Corbin, N. S., Vermeulen, D., Goetz, K. P., Jurchescu, O. D., McNeil, L. E., Bredas, J. L., **Coropceanu, V.** Vibrational Properties of Organic Donor-Acceptor Molecular Crystals: Anthracene-Pyromellitic-Dianhydride (Pmda) as a Case Study. *J. Chem. Phys.* **2015**, 143, 224503.
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