

# Chad Risiko

## List of Publications by Year in descending order

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161  
papers

8,333  
citations

38742

50  
h-index

53230

85  
g-index

170  
all docs

170  
docs citations

170  
times ranked

9783  
citing authors

| #  | ARTICLE  | IF   | CITATIONS |
|----|--|------|-----------|
| 1  | Thermomechanical enhancement of <sc>DPP&#x2013;4T</sc> through purposeful <sc>I&#x2013;conjugation</sc> disruption. Journal of Polymer Science, 2022, 60, 559-568.   | 3.8  | 5         |
| 2  | The Solution is the Solution: Data-Driven Elucidation of Solution-to-Device Feature Transfer for I&#x2013;Conjugated Polymer Semiconductors. ACS Applied Materials & Interfaces, 2022, 14, 3613-3620.                        | 8.0  | 16        |
| 3  | Unveiling the structural, electronic, and optical effects of carbon-doping on multi-layer anatase TiO <sub>2</sub> (1 0 1) and the impact on photocatalysis. Applied Surface Science, 2022, 586, 152641.                     | 6.1  | 12        |
| 4  | Computational characterization of charge transport resiliency in molecular solids. Molecular Systems Design and Engineering, 2022, 7, 651-660.   | 3.4  | 1         |
| 5  | Challenges in Information-Mining the Materials Literature: A Case Study and Perspective. Chemistry of Materials, 2022, 34, 4821-4827.  | 6.7  | 3         |
| 6  | The role of crystal packing on the optical response of trialkyltetraethynyl acenes. Journal of Chemical Physics, 2022, 157, .  | 3.0  | 3         |
| 7  | Steric Manipulation as a Mechanism for Tuning the Reduction and Oxidation Potentials of Phenothiazines. Journal of Physical Chemistry A, 2021, 125, 272-278.   | 2.5  | 9         |
| 8  | Synthesis, structures, and reactivity of isomers of [RuCp*(1,4-(Me <sub>2</sub> N) <sub>2</sub> C <sub>6</sub> H <sub>4</sub> )] <sub>2</sub> . Dalton Transactions, 2021, 50, 13020-13030.                                  | 3.3  | 3         |
| 9  | n-type charge transport in heavily p-doped polymers. Nature Materials, 2021, 20, 518-524.  | 27.5 | 66        |
| 10 | A molecular interaction&#x2013;diffusion framework for predicting organic solar cell stability. Nature Materials, 2021, 20, 525-532.   | 27.5 | 212       |
| 11 | Reactivity of an air-stable dihydrobenzoimidazole n-dopant with organic semiconductor molecules. Chem, 2021, 7, 1050-1065.   | 11.7 | 40        |
| 12 | Suppressing bias stress degradation in high performance solution processed organic transistors operating in air. Nature Communications, 2021, 12, 2352.  | 12.8 | 48        |
| 13 | OCELOT: An infrastructure for data-driven research to discover and design crystalline organic semiconductors. Journal of Chemical Physics, 2021, 154, 174705.  | 3.0  | 23        |
| 14 | Modification of the LiFePO <sub>4</sub> (010) Surface Due to Exposure to Atmospheric Gases. ACS Applied Materials & Interfaces, 2021, 13, 29034-29040.   | 8.0  | 10        |
| 15 | Evolution of Chain Dynamics and Oxidation States with Increasing Chain Length for a Donor&#x2013;Acceptor-Conjugated Oligomer Series. Macromolecules, 2021, 54, 8207-8219.   | 4.8  | 11        |
| 16 | Genetic Algorithms and Machine Learning for Predicting Surface Composition, Structure, and Chemistry: A Historical Perspective and Assessment. Chemistry of Materials, 2021, 33, 6589-6615.                                  | 6.7  | 8         |
| 17 | Lowering Electrocatalytic CO <sub>2</sub> Reduction Overpotential Using N-Annulated Perylene Diimide Rhenium Bipyridine Dyads with Variable Tether Length. Journal of the American Chemical Society, 2021, 143, 16849-16864. | 13.7 | 15        |
| 18 | What is special about silicon in functionalised organic semiconductors?. Materials Advances, 2021, 2, 5415-5421.   | 5.4  | 8         |

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|----|--|------|-----------|
| 19 | Group 14 effects in alkynyl acene small molecule semiconductors. , 2021, , .   |      | 0         |
| 20 | Reconsidering the Roles of Noncovalent Intramolecular $\pi$ - $\pi$ Locks in $\pi$ -Conjugated Molecules. Chemistry of Materials, 2021, 33, 9139-9151.   | 6.7  | 8         |
| 21 | Biotinylation as a tool to enhance the uptake of small molecules in Gram-negative bacteria. PLoS ONE, 2021, 16, e0260023.  | 2.5  | 4         |
| 22 | Nanoribbons or weakly connected acenes? The influence of pyrene insertion on linearly extended ring systems. Journal of Materials Chemistry C, 2021, 9, 16929-16934.   | 5.5  | 3         |
| 23 | Combined Computational and Experimental Approach to Determine and Understand the Solubility of Phenothiazines as Redoxmers. ECS Meeting Abstracts, 2021, MA2021-02, 1679-1679.   | 0.0  | 0         |
| 24 | Understanding the effect of host structure of nitrogen doped ultrananocrystalline diamond electrode on electrochemical carbon dioxide reduction. Carbon, 2020, 157, 408-419.   | 10.3 | 46        |
| 25 | Rational Functionalization of a C <sub>70</sub> Buckybowl To Enable a C <sub>70</sub> :Buckybowl Cocrystal for Organic Semiconductor Applications. Journal of the American Chemical Society, 2020, 142, 2460-2470.   | 13.7 | 48        |
| 26 | Nitration of benzothioxanthene: towards a new class of dyes with versatile photophysical properties. New Journal of Chemistry, 2020, 44, 900-905.  | 2.8  | 12        |
| 27 | A Genetic Algorithmic Approach to Determine the Structure of Li <sup>+</sup> Al Layered Double Hydroxides. Journal of Chemical Information and Modeling, 2020, 60, 4845-4855.  | 5.4  | 4         |
| 28 | Synthesis and electronic properties of a linearly fused anthracene dimer. Tetrahedron Letters, 2020, 61, 152182.   | 1.4  | 4         |
| 29 | Acid dyeing for green solvent processing of solvent resistant semiconducting organic thin films. Materials Horizons, 2020, 7, 2959-2969.   | 12.2 | 24        |
| 30 | Determination of the Free Energies of Mixing of Organic Solutions through a Combined Molecular Dynamics and Bayesian Statistics Approach. Journal of Chemical Information and Modeling, 2020, 60, 1424-1431.   | 5.4  | 6         |
| 31 | Exploiting Excited-State Aromaticity To Design Highly Stable Singlet Fission Materials. Journal of the American Chemical Society, 2019, 141, 13867-13876.  | 13.7 | 104       |
| 32 | Even <sup>+</sup> Odd Alkyl Chain-Length Alternation Regulates Oligothiophene Crystal Structure. Chemistry of Materials, 2019, 31, 6900-6907.  | 6.7  | 22        |
| 33 | Noncovalent Close Contacts in Fluorinated Thiophene $\pi$ -Phenylene $\pi$ -Thiophene Conjugated Units: Understanding the Nature and Dominance of O $\pi$ -H versus S $\pi$ -F and O $\pi$ -F Interactions with Respect to the Control of Polymer Conformation. Chemistry of Materials, 2019, 31, 7070-7079. | 6.7  | 23        |
| 34 | Festschrift in Honor of Prof. Jean-Luc Brédas on His 65th Birthday. Chemistry of Materials, 2019, 31, 6307-6308.   | 6.7  | 2         |
| 35 | Organic Semiconductors Derived from Dinaphtho-Fused <i>s</i> -Indacenes: How Molecular Structure and Film Morphology Influence Thin-Film Transistor Performance. Chemistry of Materials, 2019, 31, 6962-6970.  | 6.7  | 41        |
| 36 | Impact of Atomistic Substitution on Thin-Film Structure and Charge Transport in a Germanyl-ethynyl Functionalized Pentacene. Chemistry of Materials, 2019, 31, 6615-6623.  | 6.7  | 24        |

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|----|---|------|-----------|
| 37 | Enhancing CO <sub>2</sub> absorption for post-combustion carbon capture via zinc-based biomimetic catalysts in industrially relevant amine solutions. <i>International Journal of Greenhouse Gas Control</i> , 2019, 85, 156-165.       | 4.6  | 11        |
| 38 | Bis(tercarbazole) pyrene and tetrahydropyrene derivatives: photophysical and electrochemical properties, theoretical modeling, and OLEDs. <i>Journal of Materials Chemistry C</i> , 2019, 7, 5009-5018.                                 | 5.5  | 16        |
| 39 | Near-Infrared-Absorbing Indolizine-Porphyrin Push-Pull Dye for Dye-Sensitized Solar Cells. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 16474-16489.   | 8.0  | 48        |
| 40 | Triperyleno[3,3,3]propellane triimides: achieving a new generation of quasi-D <sub>3h</sub> symmetric nanostructures in organic electronics. <i>Chemical Science</i> , 2019, 10, 4951-4958.   | 7.4  | 18        |
| 41 | Deconstructing the behavior of donor-acceptor copolymers in solution & the melt: the case of PTB7. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7802-7813.  | 2.8  | 10        |
| 42 | Oxidation Pathways Involving a Sulfide-Endcapped Donor-Acceptor-Donor $\pi$ -Conjugated Molecule and Antimony(V) Chloride. <i>Journal of Physical Chemistry B</i> , 2019, 123, 3866-3874.   | 2.6  | 7         |
| 43 | Organometallic hydride-transfer agents as reductants for organic semiconductor molecules. <i>Inorganica Chimica Acta</i> , 2019, 489, 67-77.  | 2.4  | 8         |
| 44 | Chemical Stabilities of the Lowest Triplet State in Aryl Sulfones and Aryl Phosphine Oxides Relevant to OLED Applications. <i>Chemistry of Materials</i> , 2019, 31, 1507-1519.   | 6.7  | 29        |
| 45 | Solvent-Molecule Interactions Govern Crystal-Habit Selection in Naphthalene Tetracarboxylic Diimides. <i>Chemistry of Materials</i> , 2019, 31, 9691-9698.  | 6.7  | 6         |
| 46 | Computationally aided design of a high-performance organic semiconductor: the development of a universal crystal engineering core. <i>Chemical Science</i> , 2019, 10, 10543-10549.   | 7.4  | 22        |
| 47 | Positional Effects from $\delta$ -Bonded Platinum(II) on Intersystem Crossing Rates in Perylenediimide Complexes: Synthesis, Structures, and Photophysical Properties. <i>Journal of Physical Chemistry C</i> , 2018, 122, 13848-13862. | 3.1  | 18        |
| 48 | Bond Ellipticity Alternation: An Accurate Descriptor of the Nonlinear Optical Properties of $\pi$ -Conjugated Chromophores. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1377-1383.  | 4.6  | 22        |
| 49 | Delimited Polyacenes: Edge Topology as a Tool To Modulate Carbon Nanoribbon Structure, Conjugation, and Mobility. <i>Chemistry of Materials</i> , 2018, 30, 947-957.  | 6.7  | 21        |
| 50 | Effect of Halogenation on the Energetics of Pure and Mixed Phases in Model Organic Semiconductors Composed of Anthradithiophene Derivatives and C <sub>60</sub> . <i>Journal of Physical Chemistry C</i> , 2018, 122, 4757-4767.        | 3.1  | 8         |
| 51 | On the Molecular Origin of Charge Separation at the Donor-Acceptor Interface. <i>Advanced Energy Materials</i> , 2018, 8, 1702232.  | 19.5 | 51        |
| 52 | Bromination of the benzothioxanthene Bloc: toward new $\pi$ -conjugated systems for organic electronic applications. <i>Journal of Materials Chemistry C</i> , 2018, 6, 761-766.  | 5.5  | 18        |
| 53 | Impact of rotamer diversity on the self-assembly of nearly isostructural molecular semiconductors. <i>Journal of Materials Chemistry A</i> , 2018, 6, 383-394.  | 10.3 | 18        |
| 54 | Magnetic ordering in a vanadium-organic coordination polymer using a pyrrolo[2,3- <i>d</i> :5,4- <i>d'</i> ]-bis(thiazole)-based ligand. <i>RSC Advances</i> , 2018, 8, 36223-36232.  | 3.6  | 4         |

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|----|--|------|-----------|
| 55 | Exploring thermal transitions in anthradithiophene-based organic semiconductors to reveal structure-packing relationships. <i>Journal of Materials Chemistry C</i> , 2018, 6, 10924-10934.   | 5.5  | 4         |
| 56 | Presence of Short Intermolecular Contacts Screens for Kinetic Stability in Packing Polymorphs. <i>Journal of the American Chemical Society</i> , 2018, 140, 7519-7525.   | 13.7 | 29        |
| 57 | Donor or Acceptor? How Selection of the Rylene Imide End Cap Impacts the Polarity of $\pi$ -Conjugated Molecules for Organic Electronics. <i>ACS Applied Energy Materials</i> , 2018, 1, 4906-4916.  | 5.1  | 34        |
| 58 | Beyond the Hammett Effect: Using Strain to Alter the Landscape of Electrochemical Potentials. <i>ChemPhysChem</i> , 2017, 18, 2142-2146.   | 2.1  | 10        |
| 59 | Assessment of Front-Substituted Zwitterionic Cyanine Polymethines for All-Optical Switching Applications. <i>Journal of Physical Chemistry C</i> , 2017, 121, 14166-14175.   | 3.1  | 10        |
| 60 | A stable two-electron-donating phenothiazine for application in nonaqueous redox flow batteries. <i>Journal of Materials Chemistry A</i> , 2017, 5, 24371-24379.   | 10.3 | 105       |
| 61 | An unsymmetrical non-fullerene acceptor: synthesis via direct heteroarylation, self-assembly, and utility as a low energy absorber in organic photovoltaic cells. <i>Chemical Communications</i> , 2017, 53, 10168-10171.                              | 4.1  | 31        |
| 62 | Crossover from band-like to thermally activated charge transport in organic transistors due to strain-induced traps. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E6739-E6748.                  | 7.1  | 77        |
| 63 | Theory-Driven Insight into the Crystal Packing of Trialkylsilylethynyl Pentacenes. <i>Chemistry of Materials</i> , 2017, 29, 2502-2512.  | 6.7  | 30        |
| 64 | Noncovalent Interactions in Organic Electronic Materials. , 2017, , 277-302.   |      | 10        |
| 65 | Unusual Electronic Structure of the Donor-Acceptor Cocrystal Formed by Dithieno[3,2- <i>a</i> : <i>i</i> :2- <i>b</i> ,3- <i>c</i> ]phenazine and 7,7,8,8-Tetracyanoquinodimethane. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4510-4515. | 4.6  | 15        |
| 66 | Indacenodibenzothiophenes: synthesis, optoelectronic properties and materials applications of molecules with strong antiaromatic character. <i>Chemical Science</i> , 2016, 7, 5547-5558.  | 7.4  | 103       |
| 67 | Impact of Molecular Orientation and Packing Density on Electronic Polarization in the Bulk and at Surfaces of Organic Semiconductors. <i>ACS Applied Materials &amp; Interfaces</i> , 2016, 8, 14053-14062.  | 8.0  | 39        |
| 68 | Noncovalent Interactions and Impact of Charge Penetration Effects in Linear Oligoacene Dimers and Single Crystals. <i>Chemistry of Materials</i> , 2016, 28, 3990-4000.  | 6.7  | 37        |
| 69 | To bend or not to bend – are heteroatom interactions within conjugated molecules effective in dictating conformation and planarity?. <i>Materials Horizons</i> , 2016, 3, 333-339.   | 12.2 | 78        |
| 70 | Work function reduction by a redox-active organometallic sandwich complex. <i>Organic Electronics</i> , 2016, 37, 263-270.   | 2.6  | 2         |
| 71 | Understanding the Relationships Among Molecular Structure, Excited-State Properties, and Polarizabilities of $\pi$ -Conjugated Chromophores. <i>Materials and Energy</i> , 2016, , 393-419.  | 0.1  | 1         |
| 72 | High current density, long duration cycling of soluble organic active species for non-aqueous redox flow batteries. <i>Energy and Environmental Science</i> , 2016, 9, 3531-3543.  | 30.8 | 196       |

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|----|---|------|-----------|
| 73 | Packing and Disorder in Substituted Fullerenes. <i>Journal of Physical Chemistry C</i> , 2016, 120, 17242-17250.  | 3.1  | 28        |
| 74 | Polarization Energies at Organic/Organic Interfaces: Impact on the Charge Separation Barrier at Donor/Acceptor Interfaces in Organic Solar Cells. <i>ACS Applied Materials &amp; Interfaces</i> , 2016, 8, 15524-15534.       | 8.0  | 29        |
| 75 | Parallel and Perpendicular Packing in Mixed-Stack Cocrystals of Trimeric Perfluoro-ortho-phenylene Mercury and Benzo[1,2-b:6,5-b']dithiophene-4,5-dione Derivatives. <i>Crystal Growth and Design</i> , 2016, 16, 2190-2200.  | 3.0  | 3         |
| 76 | Characterizing the Polymer:Fullerene Intermolecular Interactions. <i>Chemistry of Materials</i> , 2016, 28, 1446-1452.  | 6.7  | 20        |
| 77 | Mixed-Valence Cations of Di(carbazol-9-yl) Biphenyl, Tetrahydropyrene, and Pyrene Derivatives. <i>Journal of Physical Chemistry C</i> , 2016, 120, 3156-3166.   | 3.1  | 19        |
| 78 | Strain effects on the work function of an organic semiconductor. <i>Nature Communications</i> , 2016, 7, 10270.   | 12.8 | 74        |
| 79 | Intrinsic Properties of Two Benzodithiophene-Based Donor/Acceptor Copolymers Used in Organic Solar Cells: A Quantum-Chemical Approach. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1051-1064.                         | 2.5  | 8         |
| 80 | Overcharge protection of lithium-ion batteries above 4 V with a perfluorinated phenothiazine derivative. <i>Journal of Materials Chemistry A</i> , 2016, 4, 5410-5414.  | 10.3 | 24        |
| 81 | On the impact of isomer structure and packing disorder in thienoacene organic semiconductors. <i>Journal of Materials Chemistry C</i> , 2016, 4, 4040-4048.   | 5.5  | 28        |
| 82 | Mapping the configuration dependence of electronic coupling in organic semiconductors. <i>Journal of Materials Chemistry C</i> , 2016, 4, 3825-3832.  | 5.5  | 13        |
| 83 | Noncovalent Intermolecular Interactions in Organic Electronic Materials: Implications for the Molecular Packing vs Electronic Properties of Acenes. <i>Chemistry of Materials</i> , 2016, 28, 3-16.                           | 6.7  | 215       |
| 84 | Dopants Based on Dimers of Benzimidazoline Radicals: Structures and Mechanism of Redox Reactions. <i>Chemistry - A European Journal</i> , 2015, 21, 10878-10885.  | 3.3  | 31        |
| 85 | Entanglements in P3HT and their influence on thin-film mechanical properties: Insights from molecular dynamics simulations. <i>Journal of Polymer Science, Part B: Polymer Physics</i> , 2015, 53, 934-942.                   | 2.1  | 59        |
| 86 | Distinguishing the Effects of Bond-Length Alternation versus Bond-Order Alternation on the Nonlinear Optical Properties of $\pi$ -Conjugated Chromophores. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 2158-2162. | 4.6  | 75        |
| 87 | The fate of phenothiazine-based redox shuttles in lithium-ion batteries. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 6905-6912.  | 2.8  | 40        |
| 88 | Dimers of Nineteen-Electron Sandwich Compounds: An Electrochemical Study of the Kinetics of Their Formation. <i>Organometallics</i> , 2015, 34, 3706-3712.  | 2.3  | 7         |
| 89 | Rubrene: The Interplay between Intramolecular and Intermolecular Interactions Determines the Planarization of Its Tetracene Core in the Solid State. <i>Journal of the American Chemical Society</i> , 2015, 137, 8775-8782.  | 13.7 | 56        |
| 90 | Nonlinear Optical Properties of $X(C_6H_5)_4$ ( $X = B^+, C$ ) Tj ETQq0 0 0 rgBT /Overloc<br><i>Journal of the American Chemical Society</i> , 2015, 137, 9635-9642.  | 13.7 | 21        |

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|-----|---|------|-----------|
| 91  | Molecular-Scale Understanding of Cohesion and Fracture in P3HT:Fullerene Blends. ACS Applied Materials & Interfaces, 2015, 7, 9957-9964.  | 8.0  | 60        |
| 92  | Dynamics, Miscibility, and Morphology in Polymer:Molecule Blends: The Impact of Chemical Functionality. Chemistry of Materials, 2015, 27, 7643-7651.  | 6.7  | 17        |
| 93  | Effect of Solvent Additives on the Solution Aggregation of Phenyl-C <sub>61</sub> -Butyl Acid Methyl Ester (PCBM). Chemistry of Materials, 2015, 27, 8261-8272.   | 6.7  | 26        |
| 94  | N-Substituted Phenothiazine Derivatives: How the Stability of the Neutral and Radical Cation Forms Affects Overcharge Performance in Lithium-Ion Batteries. ChemPhysChem, 2015, 16, 1179-1189.  | 2.1  | 59        |
| 95  | Heteroannulated acceptors based on benzothiadiazole. Materials Horizons, 2015, 2, 22-36.  | 12.2 | 123       |
| 96  | Theoretical description of the geometric and electronic structures of organic-organic interfaces in organic solar cells: a brief review. Science China Chemistry, 2014, 57, 1330-1339.  | 8.2  | 6         |
| 97  | Dimers of Nineteen-Electron Sandwich Compounds: Crystal and Electronic Structures, and Comparison of Reducing Strengths. Chemistry - A European Journal, 2014, 20, 15385-15394.   | 3.3  | 41        |
| 98  | Structure and Disorder in Squaraine-C <sub>60</sub> Organic Solar Cells: A Theoretical Description of Molecular Packing and Electronic Coupling at the Donor-Acceptor Interface. Advanced Functional Materials, 2014, 24, 3790-3798.      | 14.9 | 43        |
| 99  | Impact of Molecular Packing on Electronic Polarization in Organic Crystals: The Case of Pentacene vs TIPS-Pentacene. Journal of the American Chemical Society, 2014, 136, 6421-6427.  | 13.7 | 113       |
| 100 | Substrate-Induced Variations of Molecular Packing, Dynamics, and Intermolecular Electronic Couplings in Pentacene Monolayers on the Amorphous Silica Dielectric. ACS Nano, 2014, 8, 690-700.  | 14.6 | 25        |
| 101 | Ring Substituents Mediate the Morphology of PBDTPD-PCBM Bulk-Heterojunction Solar Cells. Chemistry of Materials, 2014, 26, 2299-2306.   | 6.7  | 119       |
| 102 | 25th Anniversary Article: Design of Polymethine Dyes for All-Optical Switching Applications: Guidance from Theoretical and Computational Studies. Advanced Materials, 2014, 26, 68-84.  | 21.0 | 97        |
| 103 | Interplay of alternative conjugated pathways and steric interactions on the electronic and optical properties of donor-acceptor conjugated polymers. Journal of Materials Chemistry C, 2014, 2, 8873-8879.                                | 5.5  | 25        |
| 104 | Effect of Bulky Substituents on Thiopyrylium Polymethine Aggregation in the Solid State: A Theoretical Evaluation of the Implications for All-Optical Switching Applications. Chemistry of Materials, 2014, 26, 6439-6447.                | 6.7  | 18        |
| 105 | Impact of the Nature of the Excited-State Transition Dipole Moments on the Third-Order Nonlinear Optical Response of Polymethine Dyes for All-Optical Switching Applications. ACS Photonics, 2014, 1, 261-269.                            | 6.6  | 35        |
| 106 | Influence of Molecular Shape on Solid-State Packing in Disordered PC <sub>61</sub> BM and PC <sub>71</sub> BM Fullerenes. Journal of Physical Chemistry Letters, 2014, 5, 3427-3433.  | 4.6  | 40        |
| 107 | Polymethine materials with solid-state third-order optical susceptibilities suitable for all-optical signal-processing applications. Materials Horizons, 2014, 1, 577-581.  | 12.2 | 59        |
| 108 | Impact of Bulk Aggregation on the Electronic Structure of Streptocyanines: Implications for the Solid-State Nonlinear Optical Properties and All-Optical Switching Applications. Journal of Physical Chemistry C, 2014, 118, 23575-23585. | 3.1  | 20        |

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|-----|---|------|-----------|
| 109 | Structureâ€“processingâ€“property correlations in solution-processed, small-molecule, organic solar cells. <i>Journal of Materials Chemistry C</i> , 2013, 1, 5250.   | 5.5  | 22        |
| 110 | Healing contact. <i>Nature Materials</i> , 2013, 12, 1084-1085.   | 27.5 | 2         |
| 111 | Understanding the Electronic Structure of Isoindigo in Conjugated Systems: A Combined Theoretical and Experimental Approach. <i>Macromolecules</i> , 2013, 46, 8832-8844.   | 4.8  | 63        |
| 112 | Characterization of Charge-Carrier Transport in Semicrystalline Polymers: Electronic Couplings, Site Energies, and Charge-Carrier Dynamics in Poly(bithiophene-alt-thienothiophene) [PBTTT]. <i>Journal of Physical Chemistry C</i> , 2013, 117, 1633-1640.                         | 3.1  | 92        |
| 113 | Benzo[1,2-b:6,5-bâ€™]dithiophene(dithiazole)-4,5-dione derivatives: synthesis, electronic properties, crystal packing and charge transport. <i>Journal of Materials Chemistry C</i> , 2013, 1, 1467.  | 5.5  | 23        |
| 114 | Tuning the electronic and photophysical properties of heteroleptic iridium(III) phosphorescent emitters through ancillary ligand substitution: a theoretical perspective. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 6293.  | 2.8  | 40        |
| 115 | Structural dependence of the optical properties of narrow bandgap semiconductors with orthogonal donorâ€“acceptor geometries. <i>Chemical Science</i> , 2013, 4, 1807.  | 7.4  | 34        |
| 116 | Materialsâ€“Scale Implications of Solvent and Temperature on [6,6]â€“Phenylâ€“C61â€“butyric Acid Methyl Ester (PCBM): A Theoretical Perspective. <i>Advanced Functional Materials</i> , 2013, 23, 5800-5813.  | 14.9 | 43        |
| 117 | Charge Delocalization through Benzene, Naphthalene, and Anthracene Bridges in Î€-Conjugated Oligomers: An Experimental and Quantum Chemical Study. <i>Journal of Physical Chemistry B</i> , 2013, 117, 6304-6317.   | 2.6  | 23        |
| 118 | Bis(carbazolyl) derivatives of pyrene and tetrahydropyrene: synthesis, structures, optical properties, electrochemistry, and electroluminescence. <i>Journal of Materials Chemistry C</i> , 2013, 1, 1638.  | 5.5  | 77        |
| 119 | Small Optical Gap Molecules and Polymers: Using Theory to Design More Efficient Materials for Organic Photovoltaics. <i>Topics in Current Chemistry</i> , 2013, 352, 1-38.  | 4.0  | 14        |
| 120 | Intermixing at the Pentaceneâ€“Fullerene Bilayer Interface: A Molecular Dynamics Study. <i>Advanced Materials</i> , 2013, 25, 878-882.  | 21.0 | 92        |
| 121 | Rubrene-Based Single-Crystal Organic Semiconductors: Synthesis, Electronic Structure, and Charge-Transport Properties. <i>Chemistry of Materials</i> , 2013, 25, 2254-2263.   | 6.7  | 141       |
| 122 | Electronic Polarization Effects upon Charge Injection in Oligoacene Molecular Crystals: Description via a Polarizable Force Field. <i>Journal of Physical Chemistry C</i> , 2013, 117, 13853-13860.   | 3.1  | 50        |
| 123 | nâ€“Doping of Organic Electronic Materials Using Airâ€“Stable Organometallics: A Mechanistic Study of Reduction by Dimeric Sandwich Compounds. <i>Chemistry - A European Journal</i> , 2012, 18, 14760-14772.   | 3.3  | 64        |
| 124 | Tuning Delocalization in the Radical Cations of 1,4-Bis[4-(diarylamino)styryl]benzenes, 2,5-Bis[4-(diarylamino)styryl]thiophenes, and 2,5-Bis[4-(diarylamino)styryl]pyrroles through Substituent Effects. <i>Journal of the American Chemical Society</i> , 2012, 134, 10146-10155. | 18.7 | 72        |
| 125 | Synthesis, experimental and theoretical characterization, and field-effect transistor properties of a new class of dibenzothiophene derivatives: From linear to cyclic architectures. <i>Journal of Materials Chemistry</i> , 2012, 22, 1313-1325.                                  | 6.7  | 41        |
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