Alessandro Troisi

List of Publications by Year in Descending Order

176 papers	9,785 citations	55 h-index	93 g-index
190 ext. papers	10,593 ext. citations	8.4 avg, IF	6.99 L-index

#	Paper	IF	Citations
176	Organic materials repurposing, a data set for theoretical predictions of new applications for existing compounds.. *Scientific Data*, **2022**, 9, 54	8.2	5
175	Feasibility of p-Doped Molecular Crystals as Transparent Conductive Electrodes via Virtual Screening.. *Chemistry of Materials*, **2022**, 34, 4050-4061	9.6	
174	Bright Frenkel Excitons in Molecular Crystals: A Survey. *Chemistry of Materials*, **2021**, 33, 3368-3378	9.6	5
173	Computational Identification of Novel Families of Nonfullerene Acceptors by Modification of Known Compounds. *Journal of Physical Chemistry Letters*, **2021**, 12, 5009-5015	6.4	6
172	Rapid Method for Calculating the Conformationally Averaged Electronic Structure of Conjugated Polymers. *Journal of Physical Chemistry B*, **2021**, 125, 6338-6348	3.4	6
171	Novel thermally activated delayed fluorescence materials by high-throughput virtual screening: going beyond donor□cceptor design. *Journal of Materials Chemistry C*, **2021**, 9, 3324-3333	7.1	12
170	Quantitative Prediction of the Electro-Mechanical Response in Organic Crystals. *Advanced Materials* , **2021**, 33, e2008049	24	11
169	High-throughput virtual screening for organic electronics: a comparative study of alternative strategies. *Journal of Materials Chemistry C*, **2021**, 9, 13557-13583	7.1	4
168	Determining usefulness of machine learning in materials discovery using simulated research landscapes. *Physical Chemistry Chemical Physics*, **2021**, 23, 14156-14163	3.6	6
167	Local structuring of diketopyrrolopyrrole (DPP)-based oligomers from molecular dynamics simulations. *Physical Chemistry Chemical Physics*, **2021**, 23, 19693-19707	3.6	2
166	Modeling charge transport in high-mobility molecular semiconductors: Balancing electronic structure and quantum dynamics methods with the help of experiments. *Journal of Chemical Physics*, **2020**, 152, 190902	3.9	17
165	On the Largest Possible Mobility of Molecular Semiconductors and How to Achieve It. *Advanced Functional Materials*, **2020**, 30, 2001906	15.6	22
164	Predictive Model of Charge Mobilities in Organic Semiconductor Small Molecules with Force-Matched Potentials. *Journal of Chemical Theory and Computation*, **2020**, 16, 3494-3503	6.4	10
163	Elucidating the Relationship between Multiradical Character and Predicted Singlet Fission Activity. *ChemPhotoChem*, **2020**, 4, 5223-5229	3.3	8
162	A QM/MD Coupling Method to Model the Ion-Induced Polarization of Graphene. *Journal of Chemical Theory and Computation*, **2020**, 16, 5253-5263	6.4	8
161	Relation between Local Structure, Electric Dipole, and Charge Carrier Dynamics in DHICA Melanin: A Model for Biocompatible Semiconductors. *Journal of Physical Chemistry Letters*, **2020**, 11, 1045-1051	6.4	10
160	Ethylene Glycol-Based Side Chain Length Engineering in Polythiophenes and its Impact on Organic Electrochemical Transistor Performance. *Chemistry of Materials*, **2020**, 32, 6618-6628	9.6	47

159	Exploring Charge Dissociation in a Statistical Sample of Active-Layer Models of an Organic Solar Cell. *Journal of Physical Chemistry C*, **2020**, 124, 18840-18846	3.8	3
158	Effect of Increasing the Descriptor Set on Machine Learning Prediction of Small Molecule-Based Organic Solar Cells. *Chemistry of Materials*, **2020**, 32, 7777-7787	9.6	26
157	Strategies to reduce the dynamic disorder in molecular semiconductors. *Materials Horizons*, **2020**, 7, 2922-2928	14.4	10
156	Direct probe of the nuclear modes limiting charge mobility in molecular semiconductors. *Materials Horizons*, **2019**, 6, 182-191	14.4	37
155	Exciton-Phonon Interaction Model for Singlet Fission in Prototypical Molecular Crystals. *Journal of Chemical Theory and Computation*, **2019**, 15, 3721-3729	6.4	22
154	Explaining different experimental hole mobilities: influence of polymorphism on dynamic disorder in pentacene. *Journal of Materials Chemistry C*, **2019**, 7, 9665-9670	7.1	12
153	Singlet fission molecules among known compounds: finding a few needles in a haystack. *Energy and Environmental Science*, **2019**, 12, 2412-2416	35.4	49
152	Concurrent Optimization of Organic Donor–Acceptor Pairs through Machine Learning. *Advanced Energy Materials*, **2019**, 9, 1902463	21.8	35
151	Spectroscopic signatures of quantum effects: general discussion. *Faraday Discussions*, **2019**, 221, 322-349	3.6	2
150	Quantum coherence in complex environments: general discussion. *Faraday Discussions*, **2019**, 221, 168-201	3.6	3
149	Practical Computation of the Charge Mobility in Molecular Semiconductors Using Transient Localization Theory. *Journal of Physical Chemistry C*, **2019**, 123, 6989-6997	3.8	27
148	Strong optical response and light emission from a monolayer molecular crystal. *Nature Communications*, **2019**, 10, 5589	17.4	36
147	Developing Consistent Molecular Dynamics Force Fields for Biological Chromophores via Force Matching. *Journal of Physical Chemistry B*, **2019**, 123, 428-438	3.4	14
146	Combining electronic and structural features in machine learning models to predict organic solar cells properties. *Materials Horizons*, **2019**, 6, 343-349	14.4	79
145	On the arrangement of chromophores in light harvesting complexes: chance versus design. *Faraday Discussions*, **2019**, 221, 133-149	3.6	2
144	Rapid Evaluation of Dynamic Electronic Disorder in Molecular Semiconductors. *Journal of Physical Chemistry C*, **2018**, 122, 18336-18345	3.8	26
143	Quantifying the Subtle Interplay between Intermolecular and Molecule–Substrate Interactions in Molecular Assembly on Surfaces. *Journal of Physical Chemistry C*, **2018**, 122, 17954-17962	3.8	9
142	Nonlocal Electron-Phonon Coupling in Prototypical Molecular Semiconductors from First Principles. *Journal of Chemical Theory and Computation*, **2018**, 14, 3752-3762	6.4	25

141	How fine-tuned for energy transfer is the environmental noise produced by proteins around biological chromophores?. *Physical Chemistry Chemical Physics*, **2018**, 20, 17279-17288	3.6	6
140	Sequencing conjugated polymers by eye. *Science Advances*, **2018**, 4, eaas9543	14.3	26
139	Systematic Study of the Effect of Auxiliary Acceptors in D–A–A Sensitizers Used on Dye-Sensitized Solar Cells. *Journal of Physical Chemistry C*, **2018**, 122, 23890-23898	3.8	13
138	Toward Predicting Efficiency of Organic Solar Cells via Machine Learning and Improved Descriptors. *Advanced Energy Materials*, **2018**, 8, 1801032	21.8	95
137	Trends in the electronic and geometric structure of non-fullerene based acceptors for organic solar cells. *Energy and Environmental Science*, **2017**, 10, 395-401	35.4	77
136	Effective Polarization in Pairwise Potentials at the Graphene-Electrolyte Interface. *Journal of Physical Chemistry Letters*, **2017**, 8, 703-708	6.4	43
135	How Many Parameters Actually Affect the Mobility of Conjugated Polymers?. *Physical Review Letters*, **2017**, 118, 086601	7.4	38
134	Structure-Dynamics Relation in Physically-Plausible Multi-Chromophore Systems. *Journal of Physical Chemistry Letters*, **2017**, 8, 2328-2333	6.4	11
133	Negative Isotope Effect on Field-Effect Hole Transport in Fully Substituted 13C-Rubrene. *Advanced Electronic Materials*, **2017**, 3, 1700018	6.4	26
132	Vibronic enhancement of excitation energy transport: Interplay between local and non-local exciton-phonon interactions. *Journal of Chemical Physics*, **2017**, 146, 075101	3.9	24
131	Chromophore-Dependent Intramolecular Exciton-Vibrational Coupling in the FMO Complex: Quantification and Importance for Exciton Dynamics. *Journal of Physical Chemistry B*, **2017**, 121, 10026-10035	3.4	17
130	Excitonic Coupling Modulated by Mechanical Stimuli. *Journal of Physical Chemistry Letters*, **2017**, 8, 4326-4332	6.4	6
129	Effect of Infrared Pulse Excitation on the Bound Charge-Transfer State of Photovoltaic Interfaces. *Journal of Physical Chemistry Letters*, **2017**, 8, 4872-4877	6.4	10
128	A map of high-mobility molecular semiconductors. *Nature Materials*, **2017**, 16, 998-1002	27	135
127	Importance and Nature of Short-Range Excitonic Interactions in Light Harvesting Complexes and Organic Semiconductors. *Journal of Chemical Theory and Computation*, **2017**, 13, 3754-3763	6.4	19
126	A computational study of the competing reaction mechanisms of the photo-catalytic reduction of CO on anatase(101). *Physical Chemistry Chemical Physics*, **2016**, 18, 25010-25021	3.6	12
125	Charge transport perpendicular to the high mobility plane in organic crystals: Bandlike temperature dependence maintained despite hundredfold anisotropy. *Physical Review B*, **2016**, 93,	3.3	28
124	Does the Donor–Acceptor Character of Dyes Improve the Efficiency of Dye-Sensitized Solar Cells?. *Journal of Physical Chemistry Letters*, **2016**, 7, 2989-93	6.4	9

123	Very Large Conjugation Despite Strong Nonplanarity: A Path for Designing New Semiconducting Polymers. *Journal of Physical Chemistry Letters*, **2016**, 7, 4689-4694	6.4	27
122	Reducing dynamic disorder in small-molecule organic semiconductors by suppressing large-amplitude thermal motions. *Nature Communications*, **2016**, 7, 10736	17.4	120
121	Regimes of Exciton Transport in Molecular Crystals in the Presence of Dynamic Disorder. *Advanced Functional Materials*, **2016**, 26, 2316-2325	15.6	53
120	Continuum and atomistic description of excess electrons in TiO2. *Journal of Physics Condensed Matter*, **2016**, 28, 074004	1.8	4
119	Quantum dynamics of a vibronically coupled linear chain using a surrogate Hamiltonian approach. *Journal of Chemical Physics*, **2016**, 144, 214106	3.9	6
118	Exciton Dynamics in Phthalocyanine Molecular Crystals. *Journal of Physical Chemistry C*, **2016**, 120, 7987-7996	4.8	23
117	Unexpected Like-Charge Self-Assembly of a Biguanide-Based Antimicrobial Polyelectrolyte. *Journal of Physical Chemistry Letters*, **2016**, 7, 3730-3735	6.4	9
116	Dynamics of the excitonic coupling in organic crystals. *Physical Review Letters*, **2015**, 114, 026402	7.4	87
115	Charge Dynamics in Organic Photovoltaic Materials: Interplay between Quantum Diffusion and Quantum Relaxation. *Journal of Physical Chemistry C*, **2015**, 119, 14989-14998	3.8	23
114	Excitonic couplings between molecular crystal pairs by a multistate approximation. *Journal of Chemical Physics*, **2015**, 142, 164107	3.9	18
113	Developing accurate molecular mechanics force fields for conjugated molecular systems. *Physical Chemistry Chemical Physics*, **2015**, 17, 25123-32	3.6	17
112	A very general rate expression for charge hopping in semiconducting polymers. *Journal of Chemical Physics*, **2015**, 142, 184105	3.9	24
111	Molecular Wires: Nanoscale Electrical Investigation of Layer-by-Layer Grown Molecular Wires (Adv. Mater. 11/2014). *Advanced Materials*, **2014**, 26, 1792-1792	24	
110	Nanoscale electrical investigation of layer-by-layer grown molecular wires. *Advanced Materials*, **2014**, 26, 1688-93	24	31
109	Exploiting quantum interference in dye sensitized solar cells. *ACS Nano*, **2014**, 8, 409-18	16.7	31
108	An expression for the bridge-mediated electron transfer rate in dye-sensitized solar cells. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2014**, 372, 20130011	3	3
107	Theory of charge hopping along a disordered polymer chain. *Physical Chemistry Chemical Physics*, **2014**, 16, 9997-10007	3.6	48
106	Charge Diffusion in Semiconducting Polymers: Analytical Relation between Polymer Rigidity and Time Scales for Intrachain and Interchain Hopping. *Journal of Physical Chemistry Letters*, **2014**, 5, 2637-41	6.4	40

105	Direct optical generation of long-range charge-transfer states in organic photovoltaics. *Advanced Materials*, **2014**, 26, 6163-7	24	49
104	Predicting with confidence the efficiency of new dyes in dye sensitized solar cells. *Physical Chemistry Chemical Physics*, **2014**, 16, 19106-10	3.6	19
103	Electronic Excited States in Amorphous MEH-PPV Polymers from Large-Scale First Principles Calculations. *Journal of Chemical Theory and Computation*, **2014**, 10, 1272-82	6.4	27
102	Morphology and Charge Transport in P3HT: A Theorist□ Perspective. *Advances in Polymer Science*, **2014**, 139-180	1.3	51
101	Singlet fission in linear chains of molecules. *Journal of Chemical Physics*, **2014**, 141, 204703	3.9	13
100	Narrower bands with better charge transport: the counterintuitive behavior of semiconducting copolymers. *Advanced Materials*, **2014**, 26, 7627-31	24	24
99	Modulating the Exciton Dissociation Rate by up to More than Two Orders of Magnitude by Controlling the Alignment of LUMO + 1 in Organic Photovoltaics. *Journal of Physical Chemistry C*, **2014**, 118, 27272-27280	3.8	29
98	Understanding the Microscopic Origin of the Very High Charge Mobility in PBTTT: Tolerance of Thermal Disorder. *Advanced Functional Materials*, **2014**, 24, 925-933	15.6	54
97	Relation between structure and electronic properties of amorphous MEH-PPV polymers. *Journal of the American Chemical Society*, **2013**, 135, 11247-56	16.4	56
96	Measurement of molecular motion in organic semiconductors by thermal diffuse electron scattering. *Nature Materials*, **2013**, 12, 1045-9	27	75
95	How quasi-free holes and electrons are generated in organic photovoltaic interfaces. *Faraday Discussions*, **2013**, 163, 377-92; discussion 393-432	3.6	53
94	Using Orbital Symmetry to Minimize Charge Recombination in Dye-Sensitized Solar Cells. *Angewandte Chemie*, **2013**, 125, 1007-1009	3.6	1
93	Using orbital symmetry to minimize charge recombination in dye-sensitized solar cells. *Angewandte Chemie - International Edition*, **2013**, 52, 973-5	16.4	36
92	What makes fullerene acceptors special as electron acceptors in organic solar cells and how to replace them. *Advanced Materials*, **2013**, 25, 1038-41	24	240
91	Theoretical evidence of multiple dye regeneration mechanisms in dye-sensitized solar cells. *Chemical Physics Letters*, **2013**, 570, 159-162	2.5	17
90	Charge Injection Rates in Hybrid Nanosilicon□Polythiophene Bulk Heterojunction Solar Cells. *Journal of Physical Chemistry C*, **2013**, 117, 110-115	3.8	5
89	Theory of the Charge Recombination Reaction at the Semiconductor□Adsorbate Interface in the Presence of Defects. *Journal of Physical Chemistry C*, **2013**, 117, 24196-24205	3.8	14
88	Calculation of rates of exciton dissociation into hot charge-transfer states in model organic photovoltaic interfaces. *Physical Review B*, **2013**, 88,	3.3	33

87	How TiO2 crystallographic surfaces influence charge injection rates from a chemisorbed dye sensitiser. *Physical Chemistry Chemical Physics*, **2012**, 14, 13392-401	3.6	48
86	Long-range exciton dissociation in organic solar cells. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 13498-502	11.5	138
85	Adsorption and electron injection of the N3 metal-organic dye on the TiO2 rutile (110) surface. *Physical Chemistry Chemical Physics*, **2012**, 14, 16668-76	3.6	26
84	Theoretical study of charge recombination at the TiO2-electrolyte interface in dye sensitised solar cells. *Journal of Chemical Physics*, **2012**, 137, 22A508	3.9	18
83	Evaluating Charge Recombination Rate in Dye-Sensitized Solar Cells from Electronic Structure Calculations. *Journal of Physical Chemistry C*, **2012**, 116, 7638-7649	3.8	79
82	Effect of the Anchoring Group on Electron Injection: Theoretical Study of Phosphonated Dyes for Dye-Sensitized Solar Cells. *Journal of Physical Chemistry C*, **2012**, 116, 2622-2629	3.8	82
81	What Is the Best Anchoring Group for a Dye in a Dye-Sensitized Solar Cell?. *Journal of Physical Chemistry Letters*, **2012**, 3, 1531-5	6.4	138
80	A predictive theory of charge separation in organic photovoltaics interfaces **2012**,		1
79	Chiral semiconductor phases: the optically pure D3[M(III)(S,S-EDDS)]2 (D=TTF, TSF) family. *Inorganic Chemistry*, **2011**, 50, 4039-46	5.1	6
78	Why Holes and Electrons Separate So Well in Polymer/Fullerene Photovoltaic Cells. *Journal of Physical Chemistry Letters*, **2011**, 2, 2737-2741	6.4	167
77	Dynamic disorder in molecular semiconductors: charge transport in two dimensions. *Journal of Chemical Physics*, **2011**, 134, 034702	3.9	80
76	Persistence time of charge carriers in defect states of molecular semiconductors. *Physical Chemistry Chemical Physics*, **2011**, 13, 10241-8	3.6	20
75	Hall-effect measurements probing the degree of charge-carrier delocalization in solution-processed crystalline molecular semiconductors. *Physical Review Letters*, **2011**, 107, 066601	7.4	94
74	High-Throughput Computational Screening of Chromophores for Dye-Sensitized Solar Cells. *Journal of Physical Chemistry C*, **2011**, 115, 11781-11792	3.8	110
73	Theoretical studies of dye-sensitised solar cells: from electronic structure to elementary processes. *Energy and Environmental Science*, **2011**, 4, 4473	35.4	173
72	The speed limit for sequential charge hopping in molecular materials. *Organic Electronics*, **2011**, 12, 1988-1991	3.5	45
71	Structural variability and dynamics of the P3HT/PCBM interface and its effects on the electronic structure and the charge-transfer rates in solar cells. *Physical Chemistry Chemical Physics*, **2011**, 13, 21461-70	3.6	88
70	Charge transport in high mobility molecular semiconductors: classical models and new theories. *Chemical Society Reviews*, **2011**, 40, 2347-58	58.5	343

69	Absolute Rate of Charge Separation and Recombination in a Molecular Model of the P3HT/PCBM Interface. *Journal of Physical Chemistry C*, **2011**, 115, 2406-2415	3.8	208
68	Relation between Microstructure and Charge Transport in Polymers of Different Regioregularity. *Journal of Physical Chemistry C*, **2011**, 115, 19386-19393	3.8	77
67	Quantum dynamic localization in the Holstein Hamiltonian at finite temperatures. *Physical Review B* , **2010**, 82,	3.3	11
66	Electronic Structure of TiO2 Surfaces and Effect of Molecular Adsorbates Using Different DFT Implementations. *Journal of Physical Chemistry C*, **2010**, 114, 22659-22670	3.8	112
65	Charge Transport in Self-Assembled Semiconducting Organic Layers: Role of Dynamic and Static Disorder. *Journal of Physical Chemistry C*, **2010**, 114, 10592-10597	3.8	40
64	Agent-based modeling for the 2D molecular self-organization of realistic molecules. *Journal of Physical Chemistry B*, **2010**, 114, 10151-9	3.4	10
63	Modeling the Self-Assembly of Benzenedicarboxylic Acids Using Monte Carlo and Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2010**, 114, 4376-4388	3.8	46
62	Hexagonal lattice model of the patterns formed by hydrogen-bonded molecules on the surface. *Journal of Physical Chemistry B*, **2010**, 114, 1849-58	3.4	23
61	Evaluation of the External Reorganization Energy of Polyacenes. *Journal of Physical Chemistry Letters*, **2010**, 1, 941-946	6.4	247
60	Charge transport in organic crystals: role of disorder and topological connectivity. *Journal of the American Chemical Society*, **2010**, 132, 11702-8	16.4	150
59	Theoretical Study of the Organic Photovoltaic Electron Acceptor PCBM: Morphology, Electronic Structure, and Charge Localization. *Journal of Physical Chemistry C*, **2010**, 114, 20479-20488	3.8	163
58	A method to rapidly predict the charge injection rate in dye sensitized solar cells. *Physical Chemistry Chemical Physics*, **2010**, 12, 4625-34	3.6	59
57	Organic semiconductors: impact of disorder at different timescales. *ChemPhysChem*, **2010**, 11, 2067-74	3.2	72
56	Determination of kinetic parameters of enantiomerization of benzothiadiazines by DCXplorer. *Chirality*, **2010**, 22, 789-97	2.1	11
55	Probing local electric field and conformational switching in single-molecule break junctions. *Physical Review B*, **2009**, 79,	3.3	14
54	Transition from dynamic to static disorder in one-dimensional organic semiconductors. *Journal of Chemical Physics*, **2009**, 131, 014703	3.9	36
53	Effect of the intermolecular thermal motions on the tail of the electronic density of states in polyacene crystals. *Applied Physics A: Materials Science and Processing*, **2009**, 95, 147-152	2.6	12
52	An ad hoc tight binding method to study the electronic structure of semiconducting polymers. *Chemical Physics Letters*, **2009**, 480, 210-214	2.5	29

51	Computational study of the structure and charge-transfer parameters in low-molecular-mass P3HT. *Journal of Physical Chemistry B*, **2009**, 113, 9393-401	3.4	93
50	An artificial intelligence approach for modeling molecular self-assembly: agent-based simulations of rigid molecules. *Journal of Physical Chemistry B*, **2009**, 113, 9877-85	3.4	9
49	A realistic description of the charge carrier wave function in microcrystalline polymer semiconductors. *Journal of the American Chemical Society*, **2009**, 131, 11179-86	16.4	63
48	Packing patterns of silica nanoparticles on surfaces of armored polystyrene latex particles. *Langmuir*, **2009**, 25, 12399-403	4	41
47	Charge transport in semiconductors with multiscale conformational dynamics. *Physical Review Letters*, **2009**, 102, 116602	7.4	106
46	Theories of the Charge Transport Mechanism in Ordered Organic Semiconductors. *Advances in Polymer Science*, **2009**, 213-258	1.3	5
45	Molecular structure and phase behaviour of hairy-rod polymers. *Physical Chemistry Chemical Physics* , **2009**, 11, 2105-12	3.6	22
44	Modelling charge transport in organic semiconductors: from quantum dynamics to soft matter. *Physical Chemistry Chemical Physics*, **2008**, 10, 5941-52	3.6	122
43	On the mechanism of charge transport in pentacene. *Journal of Chemical Physics*, **2008**, 129, 044704	3.9	43
42	Nuclear coupling and polarization in molecular transport junctions: beyond tunneling to function. *Science*, **2008**, 319, 1056-60	33.3	256
41	Inelastic electron tunnelling in saturated molecules with different functional groups: correlations and symmetry considerations from a computational study. *Journal of Physics Condensed Matter*, **2008**, 20, 374111	1.8	5
40	Self-assembly of sparsely distributed molecules: An efficient cluster algorithm. *Chemical Physics Letters*, **2008**, 458, 210-213	2.5	25
39	Inelastic insights for molecular tunneling pathways: bypassing the terminal groups. *Physical Chemistry Chemical Physics*, **2007**, 9, 2421-7	3.6	31
38	Single Molecule Conductance of Linear Dithioalkanes in the Liquid Phase: Apparently Activated Transport Due to Conformational Flexibility. *Journal of Physical Chemistry C*, **2007**, 111, 14567-14573	3.8	35
37	Inelastic electron tunneling spectroscopy of alkane monolayers with dissimilar attachment chemistry to gold. *Journal of the American Chemical Society*, **2007**, 129, 15303-10	16.4	24
36	Prediction of the Absolute Charge Mobility of Molecular Semiconductors: the Case of Rubrene. *Advanced Materials*, **2007**, 19, 2000-2004	24	209
35	Tracing electronic pathways in molecules by using inelastic tunneling spectroscopy. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 14255-9	11.5	88
34	Propensity rules for inelastic electron tunneling spectroscopy of single-molecule transport junctions. *Journal of Chemical Physics*, **2006**, 125, 214709	3.9	62

33	Dynamics of the intermolecular transfer integral in crystalline organic semiconductors. *Journal of Physical Chemistry A*, **2006**, 110, 4065-70	2.8	312
32	Molecular transport junctions: Propensity rules for inelastic electron tunneling spectra. *Nano Letters*, **2006**, 6, 1784-8	11.5	105
31	Charge dynamics through pi-stacked arrays of conjugated molecules: effect of dynamic disorder in different transport/transfer regimes. *Molecular Simulation*, **2006**, 32, 707-716	2	21
30	Charge-transport regime of crystalline organic semiconductors: diffusion limited by thermal off-diagonal electronic disorder. *Physical Review Letters*, **2006**, 96, 086601	7.4	473
29	Molecular signatures in the transport properties of molecular wire junctions: what makes a junction "molecular"?. *Small*, **2006**, 2, 172-81	11	111
28	Effects of hydration on molecular junction transport. *Nature Materials*, **2006**, 5, 901-8	27	104
27	Synthesis and isomerization of N-□aza-heteroaryl-□lactams. *Tetrahedron*, **2006**, 62, 12064-12070	2.4	20
26	Band structure of the four pentacene polymorphs and effect on the hole mobility at low temperature. *Journal of Physical Chemistry B*, **2005**, 109, 1849-56	3.4	152
25	Electronic Interactions and Thermal Disorder in Molecular Crystals Containing Cofacial Pentacene Units. *Chemistry of Materials*, **2005**, 17, 5024-5031	9.6	109
24	Modeling the inelastic electron tunneling spectra of molecular wire junctions. *Physical Review B*, **2005**, 72,	3.3	81
23	Self-assembly on multiple length scales: a Monte Carlo algorithm with data augmentation. *Journal of Chemical Physics*, **2005**, 122, 024102	3.9	11
22	An agent-based approach for modeling molecular self-organization. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 255-60	11.5	65
21	On the Structure and Stability of Self-Assembled Zwitterionic Peptide Amphiphiles: A Theoretical Study. *Nano Letters*, **2004**, 4, 427-431	11.5	44
20	Dynamic nature of the intramolecular electronic coupling mediated by a solvent molecule: a computational study. *Journal of the American Chemical Society*, **2004**, 126, 2215-24	16.4	57
19	All-Atom Numerical Studies of Self-Assembly of Zwitterionic Peptide Amphiphiles. *Journal of Physical Chemistry B*, **2004**, 108, 15278-15284	3.4	41
18	Conformational Molecular Rectifiers. *Nano Letters*, **2004**, 4, 591-595	11.5	124
17	Modulating charge-transfer interactions in topologically different porphyrin-C60 dyads. *Chemistry - A European Journal*, **2003**, 9, 4968-79	4.8	102
16	Construction of electronic diabatic states within a molecular orbital scheme. *Journal of Chemical Physics*, **2003**, 118, 5356-5363	3.9	18

15	Vibronic effects in off-resonant molecular wire conduction. *Journal of Chemical Physics*, **2003**, 118, 6072-6082	3.9	119
14	A rate constant expression for charge transfer through fluctuating bridges. *Journal of Chemical Physics*, **2003**, 119, 5782-5788	3.9	121
13	Molecular rectification through electric field induced conformational changes. *Journal of the American Chemical Society*, **2002**, 124, 14528-9	16.4	88
12	Hole Migration in DNA:a Theoretical Analysis of the Role of Structural Fluctuations. *Journal of Physical Chemistry B*, **2002**, 106, 2093-2101	3.4	201
11	Structure and photophysics of an old, new molecule: 1,3,6,8-tetraazatricyclo[4.4.1.1(3,8)]dodecane. *Journal of the American Chemical Society*, **2002**, 124, 149-58	16.4	9
10	A quantum-mechanical description of macrocyclic ring rotation in benzylic amide. *Chemistry - A European Journal*, **2001**, 7, 1450-4	4.8	24
9	The hole transfer in DNA: calculation of electron coupling between close bases. *Chemical Physics Letters*, **2001**, 344, 509-518	2.5	181
8	Parallel (face-to-face) versus perpendicular (edge-to-face) alignment of electron donors and acceptors in fullerene porphyrin dyads: the importance of orientation in electron transfer. *Journal of the American Chemical Society*, **2001**, 123, 9166-7	16.4	142
7	Reducing Molecular Shuttling to a Single Dimension. *Angewandte Chemie*, **2000**, 112, 358-361	3.6	27
6	Reducing Molecular Shuttling to a Single Dimension. *Angewandte Chemie - International Edition*, **2000**, 39, 350-353	16.4	65
5	Valencies of a small fullerene: structures and energetics of C24H2m. *Chemical Physics Letters*, **1999**, 312, 77-84	2.5	18
4	The heptakisoctahedral group and its relevance to carbon allotropes with negative curvature. *Journal of Mathematical Chemistry*, **1999**, 26, 101-123	2.1	24
3	Independent sets and the prediction of addition patterns for higher fullerenes. *Journal of the Chemical Society Perkin Transactions II*, **1999**, 2023-2027		12
2	Simulation of STM Images from Commercially Available Software. *Journal of the American Chemical Society*, **1999**, 121, 5392-5395	16.4	19
1	Performance Prediction and Experimental Optimization Assisted by Machine Learning for Organic Photovoltaics. *Advanced Intelligent Systems*,2100261	6	2