B Baumeier

List of Publications by Year
in descending order

52	2,289	304743	206112
papers	citations	22 h-index	48 g-index

65	65	65	2788
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Microscopic Simulations of Charge Transport in Disordered Organic Semiconductors. Journal of Chemical Theory and Computation, 2011, 7, 3335-3345.	5.3	345
2	Density-functional based determination of intermolecular charge transfer properties for large-scale morphologies. Physical Chemistry Chemical Physics, 2010, 12, 11103.	2.8	222
3	Structural, elastic, and electronic properties of SiC, BN, and BeO nanotubes. Physical Review B, 2007, 76, .	3.2	211
4	Impact of mesoscale order on open-circuit voltage in organic solar cells. Nature Materials, 2015, 14, 434-439.	27.5	184
5	Charge Transport in Organic Crystals: Role of Disorder and Topological Connectivity. Journal of the American Chemical Society, 2010, 132, 11702-11708.	13.7	157
6	Frenkel and Charge-Transfer Excitations in Donorâ€“acceptor Complexes from Many-Body Greenâ€™s Functions Theory. Journal of Chemical Theory and Computation, 2012, 8, 2790-2795.	5.3	98
7	Excited States of Dicyanovinyl-Substituted Oligothiophenes from Many-Body Greenâ€™s Functions Theory. Journal of Chemical Theory and Computation, 2012, 8, 997-1002.	5.3	86
8	Design Rules for Charge-Transport Efficient Host Materials for Phosphorescent Organic Light-Emitting Diodes. Journal of the American Chemical Society, 2012, 134, 13818-13822.	13.7	85
9	Comparative Study of Microscopic Charge Dynamics in Crystalline Acceptor-Substituted Oligothiophenes. Journal of the American Chemical Society, 2012, 134, 6052-6056.	13.7	78
10	Challenges for in silico design of organic semiconductors. Journal of Materials Chemistry, 2012, 22, 10971.	6.7	57
11	Can Lattice Models Predict the Density of States of Amorphous Organic Semiconductors?. Physical Review Letters, 2012, 109, 136401.	7.8	55
12	Electronic Excitations in Pushâ€“Pull Oligomers and Their Complexes with Fullerene from Many-Body Greenâ€™s Functions Theory with Polarizable Embedding. Journal of Chemical Theory and Computation, 2014, 10, 3104-3110.	5.3	55
13	Stochastic modeling of molecular charge transport networks. Physical Review B, 2012, 86, .	3.2	48
14	Cloaking from Surface Plasmon Polaritons by a Circular Array of Point Scatterers. Physical Review Letters, 2009, 103, 246803.	7.8	40
15	Bulk and surface electronic structures of alkaline-earth metal oxides: Bound surface and image-potential states from first principles. Physical Review B, 2007, 76, .	3.2	38
16	Toward Quantitative Structureâ€“Property Relationships for Charge Transfer Rates of Polycyclic Aromatic Hydrocarbons. Journal of Chemical Theory and Computation, 2011, 7, 2549-2555.	5.3	37
17	Self-interaction-corrected pseudopotentials for silicon carbide. Physical Review B, 2006, 73, .	3.2	34
18	Atomic and electronic structure ofBeOand theBeO(101Â¯0)surface: Anab initioinvestigation. Physical Review B, 2007, 75, .	3.2	34

#	Article	IF	Citations
19	Electronic Excitations in Complex Molecular Environments: Many-Body Greenâ€™s Functions Theory in VOTCA-XTP. Journal of Chemical Theory and Computation, 2018, 14, 6253-6268.	5.3	28
20	Electronic structure of alkali-metal fluorides, oxides, and nitrides: Density-functional calculations including self-interaction corrections. Physical Review B, 2008, 78, .	3.2	27
21	Parametrization of Extended Gaussian Disorder Models from Microscopic Charge Transport Simulations. Journal of Chemical Theory and Computation, 2014, 10, 2508-2513.	5.3	27
22	Evolutionary Approach to Constructing a Deep Feedforward Neural Network for Prediction of Electronic Coupling Elements in Molecular Materials. Journal of Chemical Theory and Computation, 2019, 15, 1777-1784.	5.3	27
23	Improved general-purpose five-point model for water: TIP5P/2018. Journal of Chemical Physics, 2018, 149, 224507.	3.0	23
24	Transmission of light through a thin metal film with periodically and randomly corrugated surfaces. Journal of Optics, 2006, 8, S191-S207.	1.5	21
25	Excited-state electronic structure of molecules using many-body Greenâ€™s functions: Quasiparticles and electronâ€“hole excitations with VOTCA-XTP. Journal of Chemical Physics, 2020, 152, 114103.	3.0	20
26	Two Channels of Charge Generation in Perylene Monoimide Solidâ€State Dyeâ€Sensitized Solar Cells. Advanced Energy Materials, 2014, 4, 1300640.	19.5	18
27	First-principles investigation of an epitaxial silicon oxynitride layer on a<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>6</mml:mn><mml:mi>H</mml:mi><mml:mtext>â€</mml:mtext><mml:mi mathvariant="normal">Si</mml:mi><mml:mi mathvariant="normal">C</mml:mi><mml:mrow><mml:mo>(</mml:mo><mml:mn>0001</mml:mn><mml:mo>)</mml:mo></mml:mrow></mml:mrow Physical Review B, 2008, 77, .	3.2	16
28	Charge transport in columnar mesophases of carbazole macrocycles. Journal of Chemical Physics, 2010, 133, 134901.	3.0	16
29	Excited-State Geometry Optimization of Small Molecules with Many-Body Greenâ€™s Functions Theory. Journal of Chemical Theory and Computation, 2021, 17, 879-888.	5.3	16
30	The Goos-HÃnchen effect for surface plasmon polaritons. Optics Express, 2011, 19, 15483.	3.4	14
31	Observing Charge Dynamics in Surface Reactions by Time-Resolved Stark Effects. Journal of Physical Chemistry C, 2013, 117, 9171-9177.	3.1	14
32	Insights into the Kinetics of Supramolecular Comonomer Incorporation in Water. Macromolecules, 2019, 52, 3049-3055.	4.8	14
33	A General Framework for Consistent Estimation of Charge Transport Properties via Random Walks in Random Environments. Multiscale Modeling and Simulation, 2014, 12, 1108-1134.	1.6	13
34	Intermolecular Singlet and Triplet Exciton Transfer Integrals from Many-Body Greenâ€™s Functions Theory. Journal of Chemical Theory and Computation, 2017, 13, 1584-1594.	5.3	13
35	Efficient Simulation of Markov Chains Using Segmentation. Methodology and Computing in Applied Probability, 2014, 16, 465-484.	1.2	11
36	Ultrafast Formation of the Charge Transfer State of Prodan Reveals Unique Aspects of the Chromophore Environment. Journal of Physical Chemistry B, 2020, 124, 2643-2651.	2.6	11

#	Article	IF	Citations
37	Wasserstein metric for improved quantum machine learning with adjacency matrix representations. Machine Learning: Science and Technology, 2020, 1, 03LT01.	5.0	11
38	Getting excited: challenges in quantum-classical studies of excitons in polymeric systems. Physical Chemistry Chemical Physics, 2016, 18, 30297-30304.	2.8	10
39	Glassy dynamics from generalized mode-coupling theory: existence and uniqueness of solutions for hierarchically coupled integro-differential equations. Journal of Statistical Mechanics: Theory and Experiment, 2020, 2020, 103301.	2.3	9
40	First-principles investigation of the atomic and electronic structure of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		