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	Ab initio modeling of excitons: from perfect crystals to biomaterials. Advances in Physics: X, 2021, 6, .	4.1	4
2	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
3	Jamming and force distribution in growing epithelial tissue. Physical Review Research, 2021, 3, .	3.6	4
4	Machine Learning of Quasiparticle Energies in Molecules and Clusters. Journal of Chemical Theory and Computation, 2021, 17, 4891-4900.	5.3	6
5	Coarse-grained modeling of cell division in 3D: influence of density, medium viscosity, and inter-membrane friction on cell growth and nearest neighbor distribution. Soft Materials, 2020, 18, 150-162.	1.7	3
6	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
7	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
8	Multiscale simulations of singlet and triplet exciton dynamics in energetically disordered molecular systems based on many-body Green's functions theory. New Journal of Physics, 2020, 22, 033033.	2.9	4
9	Development and Testing of an All-Atom Force Field for Diketopyrrolopyrrole Polymers with Conjugated Substituents. Journal of Physical Chemistry B, 2020, 124, 11030-11039.	2.6	6
10	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
11	Wasserstein metric for improved quantum machine learning with adjacency matrix representations. Machine Learning: Science and Technology, 2020, 1, 03LT01.	5.0	11
12	Quantitative predictions of photoelectron spectra in amorphous molecular solids from multiscale quasiparticle embedding. Physical Review B, 2020, 101, .	3.2	8
13	Backbone Chemical Composition and Monomer Sequence Effects on Phenylene Polymer Persistence Lengths. Macromolecules, 2019, 52, 5307-5316.	4.8	4
14	Insights into the Kinetics of Supramolecular Comonomer Incorporation in Water. Macromolecules, 2019, 52, 3049-3055.	4.8	14
15	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
16	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
17	Improved general-purpose five-point model for water: TIP5P/2018. Journal of Chemical Physics, 2018, 149, 224507.	3.0	23
18	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

#	Article	IF	Citations
19	Solvent effects on optical excitations of poly para phenylene ethynylene studied by QM/MM simulations based on many-body Green's functions theory. European Physical Journal: Special Topics, 2016, 225, 1743-1756.	2.6	6
20	Getting excited: challenges in quantum-classical studies of excitons in polymeric systems. Physical Chemistry Chemical Physics, 2016, 18, 30297-30304.	2.8	10
21	Impact of mesoscale order on open-circuit voltage in organic solar cells. Nature Materials, 2015, 14, 434-439.	27.5	184
22	Efficient Simulation of Markov Chains Using Segmentation. Methodology and Computing in Applied Probability, 2014, 16, 465-484.	1.2	11
23	Two Channels of Charge Generation in Perylene Monoimide Solidâ€State Dyeâ€Sensitized Solar Cells. Advanced Energy Materials, 2014, 4, 1300640.	19.5	18
24	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
25	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
26	Parametrization of Extended Gaussian Disorder Models from Microscopic Charge Transport Simulations. Journal of Chemical Theory and Computation, 2014, 10, 2508-2513.	5.3	27
27	Observing Charge Dynamics in Surface Reactions by Time-Resolved Stark Effects. Journal of Physical Chemistry C, 2013, 117, 9171-9177.	3.1	14
28	Efficient simulation of charge transport in deep-trap media. , 2012, , .		3
29	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
30	Challenges for in silico design of organic semiconductors. Journal of Materials Chemistry, 2012, 22, 10971.	6.7	57
31	Stochastic modeling of molecular charge transport networks. Physical Review B, 2012, 86, .	3.2	48
32	Can Lattice Models Predict the Density of States of Amorphous Organic Semiconductors?. Physical Review Letters, 2012, 109, 136401.	7.8	55
33	Comparative Study of Microscopic Charge Dynamics in Crystalline Acceptor-Substituted Oligothiophenes. Journal of the American Chemical Society, 2012, 134, 6052-6056.	13.7	78
34	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
35	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
36	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

#	Article	IF	Citations
37	Scattering of surface-plasmon polaritons by a localized dielectric surface defect studied using an effective boundary condition. Physical Review A, 2011, 84, .	2.5	8
38	Microscopic Simulations of Charge Transport in Disordered Organic Semiconductors. Journal of Chemical Theory and Computation, 2011, 7, 3335-3345.	5.3	345
39	The Goos-HÃnchen effect for surface plasmon polaritons. Optics Express, 2011, 19, 15483.	3.4	14
40	The Goos-HÃnchen effect for surface plasmon polaritons: erratum. Optics Express, 2011, 19, 18807.	3.4	1
41	Charge transport in columnar mesophases of carbazole macrocycles. Journal of Chemical Physics, 2010, 133, 134901.	3.0	16
42	Density-functional based determination of intermolecular charge transfer properties for large-scale morphologies. Physical Chemistry Chemical Physics, 2010, 12, 11103.	2.8	222
43	Charge Transport in Organic Crystals: Role of Disorder and Topological Connectivity. Journal of the American Chemical Society, 2010, 132, 11702-11708.	13.7	157
44	Cloaking from Surface Plasmon Polaritons by a Circular Array of Point Scatterers. Physical Review Letters, 2009, 103, 246803.	7.8	40
45	Electronic structure of alkali-metal fluorides, oxides, and nitrides: Density-functional calculations including self-interaction corrections. Physical Review B, 2008, 78, .	3.2	27
46	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>	3.2	16
47	Physical Review B, 2009, 79, . xmlns:mml="http://www.w3.org/1998/Math/MathML"		