Harald Oberhofer

List of Publications by Year
in descending order

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63	3,164	186265	155660
papers	citations	28 h-index	55 g-index

65	65	65	3764
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	1.1	445
2	Charge Transport in Molecular Materials: An Assessment of Computational Methods. Chemical Reviews, 2017, 117, 10319-10357.	47.7	310
3	Electronic couplings for molecular charge transfer: Benchmarking CDFT, FODFT, and FODFTB against high-level ab initio calculations. Journal of Chemical Physics, 2014, 140, 104105.	3.0	175
4	Chemical Activity of Thin Oxide Layers: Strong Interactions with the Support Yield a New Thinâ€Film Phase of ZnO. Angewandte Chemie - International Edition, 2013, 52, 11925-11929.	13.8	158
5	Biased Sampling of Nonequilibrium Trajectories:Â Can Fast Switching Simulations Outperform Conventional Free Energy Calculation Methods?â€. Journal of Physical Chemistry B, 2005, 109, 6902-6915.	2.6	151
6	Electronic couplings for molecular charge transfer: benchmarking CDFT, FODFT and FODFTB against high-level ab initio calculations. II. Physical Chemistry Chemical Physics, 2015, 17, 14342-14354.	2.8	119
7	Charge constrained density functional molecular dynamics for simulation of condensed phase electron transfer reactions. Journal of Chemical Physics, 2009, 131, 064101.	3.0	96
8	Electronic coupling matrix elements from charge constrained density functional theory calculations using a plane wave basis set. Journal of Chemical Physics, 2010, 133, 244105.	3.0	95
9	Photoswitching in nanoporous, crystalline solids: an experimental and theoretical study for azobenzene linkers incorporated in MOFs. Physical Chemistry Chemical Physics, 2015, 17, 14582-14587.	2.8	91
10	Surface Adsorption Energetics Studied with â€œGold Standardâ€•Wave-Function-Based Ab Initio Methods: Small-Molecule Binding to TiO₂(110). Journal of Physical Chemistry Letters, 2016, 7, 4207-4212.	4.6	86
11	Implicit Solvation Methods for Catalysis at Electrified Interfaces. Chemical Reviews, 2022, 122, 10777-10820.	47.7	82
12	Virtual Screening for High Carrier Mobility in Organic Semiconductors. Journal of Physical Chemistry Letters, 2016, 7, 3973-3977.	4.6	78
13	Revisiting electronic couplings and incoherent hopping models for electron transport in crystalline C60 at ambient temperatures. Physical Chemistry Chemical Physics, 2012, 14, 13846.	2.8	77
14	Prediction of Reorganization Free Energies for Biological Electron Transfer: A Comparative Study of Ru-Modified Cytochromes and a 4-Helix Bundle Protein. Journal of the American Chemical Society, 2010, 132, 17032-17040.	13.7	76
15	Equilibrium free energies from fast-switching trajectories with large time steps. Journal of Chemical Physics, 2006, 124, 044113.	3.0	66
16	Active discovery of organic semiconductors. Nature Communications, 2021, 12, 2422.	12.8	66
17	Function-Space-Based Solution Scheme for the Size-Modified Poissonâ€“Boltzmann Equation in Full-Potential DFT. Journal of Chemical Theory and Computation, 2016, 12, 4052-4066.	5.3	63
18	On the Inapplicability of Electron-Hopping Models for the Organic Semiconductor Phenyl-C61-butyric Acid Methyl Ester (PCBM). Journal of Physical Chemistry Letters, 2013, 4, 1012-1017.	4.6	61

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19	Insight into the Mechanism of the Ru²⁺â€“Ru³⁺ Electron Selfâ€Exchange Reaction from Quantitative Rate Calculations. Angewandte Chemie - International Edition, 2010, 49, 3631-3634.	13.8	53
20	Atomic structures and orbital energies of 61,489 crystal-forming organic molecules. Scientific Data, 2020, 7, 58.	5.3	52
21	Perspective: On the active site model in computational catalyst screening. Journal of Chemical Physics, 2017, 146, 040901.	3.0	48
22	Intricacies of DFT+U, Not Only in a Numeric Atom Centered Orbital Framework. Journal of Chemical Theory and Computation, 2019, 15, 1705-1718.	5.3	41
23	First-Principles Free-Energy Barriers for Photoelectrochemical Surface Reactions: Proton Abstraction at <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>TiO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub><mml:mo stretchy="false">(</mml:mo><mml:mn>110</mml:mn><mml:mo) Tj ET Q q 1 1 0.784314 rg BT /Overlock 10 Tf 50 567 Td (stretchy="false")	7.8	40
24	Embedded-cluster calculations in a numeric atomic orbital density-functional theory framework. Journal of Chemical Physics, 2014, 141, 024105.	3.0	38
25	Finding the Right Bricks for Molecular Legos: A Data Mining Approach to Organic Semiconductor Design. Chemistry of Materials, 2019, 31, 969-978.	6.7	38
26	Transferable ionic parameters for first-principles Poisson-Boltzmann solvation calculations: Neutral solutes in aqueous monovalent salt solutions. Journal of Chemical Physics, 2017, 146, 134103.	3.0	37
27	Critical analysis of fragment-orbital DFT schemes for the calculation of electronic coupling values. Journal of Chemical Physics, 2016, 144, 054103.	3.0	36
28	Generalized molecular solvation in non-aqueous solutions by a single parameter implicit solvation scheme. Journal of Chemical Physics, 2019, 150, 041710.	3.0	31
29	Efficient Implicit Solvation Method for Full Potential DFT. Journal of Chemical Theory and Computation, 2017, 13, 5582-5603.	5.3	30
30	Thermal and Electronic Fluctuations of Flexible Adsorbed Molecules: Azobenzene on Ag(111). Physical Review Letters, 2016, 116, 146101.	7.8	26
31	Proton Transfer Drives Protein Radical Formation in Helicobacter pylori Catalase but Not in Penicillium vitale Catalase. Journal of the American Chemical Society, 2011, 133, 4285-4298.	13.7	25
32	First-principles embedded-cluster calculations of the neutral and charged oxygen vacancy at the rutile<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>(110) surface. Physical Review B, 2015, 92, .	3.2	25
33	Single molecule pulling with large time steps. Physical Review E, 2007, 75, 061106.	2.1	23
34	Cooperative Large-Hysteresis Spin-Crossover Transition in the Iron(II) Triazolate [Fe(ta)₂] Metalâ€“Organic Framework. Inorganic Chemistry, 2020, 59, 10501-10511.	4.0	23
35	Gas-phase formation of large neutral alkaline-earth metal tryptophan complexes. Journal of the American Society for Mass Spectrometry, 2008, 19, 1021-1026.	2.8	22
36	Genarris: Random generation of molecular crystal structures and fast screening with a Harris approximation. Journal of Chemical Physics, 2018, 148, 241701.	3.0	21

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37	Sizeâ€Extensive Molecular Machine Learning with Global Representations. ChemSystemsChem, 2020, 2, e1900052.	2.6	20
38	Optimum bias for fast-switching free energy calculations. Computer Physics Communications, 2008, 179, 41-45.	7.5	18
39	First-principles thermodynamic screening approach to photo-catalytic water splitting with co-catalysts. Journal of Chemical Physics, 2013, 139, 044710.	3.0	18
40	Efficient extraction of free energy profiles from nonequilibrium experiments. Journal of Computational Chemistry, 2009, 30, 1726-1736.	3.3	16
41	Knowledge discovery through chemical space networks: the case of organic electronics. Journal of Molecular Modeling, 2019, 25, 87.	1.8	14
42	Electrocatalysis Beyond the Computational Hydrogen Electrode. , 2020, , 1505-1537.		14
43	Towards a transferable design of solid-state embedding models on the example of a rutile TiO2 (110) surface. Journal of Chemical Physics, 2019, 151, 184114.	3.0	12
44	Improved Projection-Operator Diabatization Schemes for the Calculation of Electronic Coupling Values. Journal of Chemical Theory and Computation, 2020, 16, 7431-7443.	5.3	12
45	Recent advances of multiphoton absorption in metalâ€“organic frameworks. Journal of Materials Chemistry C, 2022, 10, 6912-6934.	5.5	12
46	Consecutive reactions of small, free tantalum clusters with dioxygen controlled by relaxation dynamics. Physical Chemistry Chemical Physics, 2017, 19, 5985-5993.	2.8	11
47	Aspects of semiconductivity in soft, porous metal-organic framework crystals. Journal of Chemical Physics, 2019, 151, 015102.	3.0	11
48	Mobile Small Polarons Qualitatively Explain Conductivity in Lithium Titanium Oxide Battery Electrodes. Journal of Physical Chemistry Letters, 2020, 11, 2535-2540.	4.6	11
49	Photoelectron angular distributions as sensitive probes of surfactant layer structure at the liquidâ€“vapor interface. Physical Chemistry Chemical Physics, 2022, 24, 4796-4808.	2.8	11
50	Comment on â€œA centroid molecular dynamics study of liquid para hydrogen and ortho deuteriumâ€•[J. Chem. Phys. 121, 6412 (2004)]. Journal of Chemical Physics, 2005, 122, 057101.	3.0	10
51	Electrocatalysis Beyond the Computational Hydrogen Electrode. , 2018, , 1-33.		10
52	Correction to â€œInapplicability of Electron-Hopping Models for the Organic Semiconductor Phenyl-C61-butyric Acid Methyl Ester (PCBM)â€• Journal of Physical Chemistry Letters, 2014, 5, 2765-2766.	4.6	9
53	Formation and stability of small polarons at the lithium-terminated Li4Ti5O12 (LTO) (111) surface. Journal of Chemical Physics, 2020, 153, 144701.	3.0	7
54	Response properties at the dynamic water/dichloroethane liquidâ€“liquid interface. Molecular Physics, 2018, 116, 3409-3416.	1.7	6

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55	Toward First-Principles-Level Polarization Energies in Force Fields: A Gaussian Basis for the Atom-Condensed Kohnâ€“Sham Method. Journal of Chemical Theory and Computation, 2019, 15, 4516-4525.	5.3	6
56	An Iterative Fragment Scheme for the ACKS2 Electronic Polarization Model: Application to Molecular Dimers and Chains. Journal of Chemical Theory and Computation, 2020, 16, 5723-5735.	5.3	6
57	Large timeâ€step, fastâ€switching free energy calculations with nonâ€symplectic integrators. Israel Journal of Chemistry, 2007, 47, 215-223.	2.3	4
58	Anomalous pressure dependence of the electronic properties of molecular crystals explained by changes in intermolecular electronic coupling. Synthetic Metals, 2019, 253, 9-19.	3.9	4
59	Polaron-Assisted Charge Transport in Li-Ion Battery Anode Materials. ACS Applied Energy Materials, 2021, 4, 8583-8591.	5.1	4
60	Piecewise Multipole-Expansion Implicit Solvation for Arbitrarily Shaped Molecular Solutes. Journal of Chemical Theory and Computation, 2022, 18, 461-478.	5.3	2
61	Electronic property trends of single-component organic molecular crystals containing C, N, O, and H. Computational Materials Science, 2021, 197, 110510.	3.0	1
62	Interfacial Charge Transfer Influences Thin-Film Polymorphism. Journal of Physical Chemistry C, 2022, 126, 2868-2876.	3.1	1
63	Combining Theory and Experiments To Study the Influence of Gas Sorption on the Conductivity Properties of Metalâ€“Organic Frameworks. ACS Applied Materials & Interfaces, 2022, 14, 33662-33674.	8.0	1