

Sebastian Metz

List of Publications by Year in descending order

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Version: 2024-02-01

24
papers

953
citations

758635

12
h-index

642321

23
g-index

24
all docs

24
docs citations

24
times ranked

1344
citing authors

#	ARTICLE	IF	CITATIONS
1	<sc>C</sc>hem<sc>S</sc>hellâ€”a modular software package for <sc>QM</sc>/<sc>MM</sc> simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 101-110.	6.2	351
2	DL_MESO: highly scalable mesoscale simulations. Molecular Simulation, 2013, 39, 796-821.	0.9	123
3	Crossing the Valley of Death: From Fundamental to Applied Research in Electrolysis. JACS Au, 2021, 1, 527-535.	3.6	79
4	A Combined QM/MM Study on the Reductive Half-Reaction of Xanthine Oxidase: Substrate Orientation and Mechanism. Journal of the American Chemical Society, 2009, 131, 14885-14902.	6.6	70
5	On the influence of the anodic porous transport layer on PEM electrolysis performance at high current densities. International Journal of Hydrogen Energy, 2020, 45, 6047-6058.	3.8	53
6	Theoretical studies on the reactivity of molybdenum enzymes. Coordination Chemistry Reviews, 2011, 255, 1085-1103.	9.5	50
7	Reductive Half-Reaction of Aldehyde Oxidoreductase toward Acetaldehyde: A Combined QM/MM Study. Journal of the American Chemical Society, 2009, 131, 4628-4640.	6.6	38
8	Reductive half-reaction of aldehyde oxidoreductase toward acetaldehyde: Ab initio and free energy quantum mechanical/molecular mechanical calculations. Journal of Chemical Physics, 2010, 132, 035101.	1.2	33
9	QM/MM Studies of Xanthine Oxidase: Variations of Cofactor, Substrate, and Active-Site Glu802. Journal of Physical Chemistry B, 2010, 114, 1506-1517.	1.2	29
10	N₂O Formation via Reductive Disproportionation of NO by Mononuclear Copper Complexes: A Mechanistic DFT Study. Inorganic Chemistry, 2017, 56, 3820-3833.	1.9	25
11	Accuracy of Hybrid Functionals with Non-Self-Consistent Kohnâ€”Sham Orbitals for Predicting the Properties of Semiconductors. Journal of Chemical Theory and Computation, 2020, 16, 3543-3557.	2.3	17
12	Chloro Complexes with Nitrogen Donors. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2006, 632, 814-818.	0.6	15
13	Understanding the Swelling Behavior of Modified Nanoclay Filler Particles in Water and Ethanol. Journal of Physical Chemistry C, 2015, 119, 12625-12642.	1.5	12
14	Thermodynamics, Electronic Structure, and Vibrational Properties of Snn(Slâ€”xSex)m Solid Solutions for Energy Applications. Chemistry of Materials, 2019, 31, 3672-3685.	3.2	11
15	Cooperative Modes of Action of Antimicrobial Peptides Characterized with Atomistic Simulations: A Study on Cecropin B. Journal of Physical Chemistry B, 2018, 122, 5908-5921.	1.2	10
16	Control of the dipole layer of polar organic molecules adsorbed on metal surfaces via different charge-transfer channels. Physical Review B, 2017, 95, .	1.1	8
17	Monte Carlo simulations of gadolinium doped ceria surfaces. Solid State Ionics, 2018, 324, 128-137.	1.3	8
18	Graphene-based acceptor molecules for organic photovoltaic cells: a predictive study identifying high modularity and morphological stability. RSC Advances, 2016, 6, 13653-13656.	1.7	6

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19	Targeting ideal acceptor-donor materials based on hexabenzocoronene. <i>Journal of Molecular Structure</i> , 2018, 1161, 442-452.	1.8	5
20	Novel benzothiazole half-squaraines: model chromophores to study dye-TiO ₂ interactions in dye-sensitized solar cells. <i>Journal of Materials Chemistry A</i> , 2020, 8, 22191-22205.	5.2	4
21	A perspective on using experiment and theory to identify design principles in dye-sensitized solar cells. <i>Science and Technology of Advanced Materials</i> , 2018, 19, 599-612.	2.8	3
22	A combined experimental/theoretical approach to accelerated fuel cell development by quantitative prediction of redox potentials. <i>Journal of Power Sources</i> , 2018, 399, 443-447.	4.0	2
23	Using irradiation effect to study the disparate anchoring stabilities of polar-organic molecules adsorbed on bulk and thin-film metal surfaces. <i>Applied Surface Science</i> , 2019, 493, 1090-1097.	3.1	1
24	An ab initio characterization of the electronic structure of LaCo _x Fe _{1-x} O ₃ for x = 0.5. <i>Physica Status Solidi (B): Basic Research</i> , 2016, 253, 1673-1687.	0.7	0