# Sebastian Metz

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8144853/publications.pdf

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| 24 | 953 | 758635 12 | 642321 23 |
|---|---|---|---|
| papers | citations | h-index | g-index |

| 24 | 24 | 24 | 1344 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Crossing the Valley of Death: From Fundamental to Applied Research in Electrolysis. Jacs Au, 2021, 1, 527-535. | 3.6 | 79 |
| 2 | Novel benzothiazole half-squaraines: model chromophores to study dyeâ€“TiO<sub>2</sub>interactions in dye-sensitized solar cells. Journal of Materials Chemistry A, 2020, 8, 22191-22205. | 5.2 | 4 |
| 3 | 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 |
| 4 | 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 |
| 5 | Using irradiation effect to study the disparate anchoring stabilities of polar-organic molecules adsorbed on bulk and thin-film metal surfaces. Applied Surface Science, 2019, 493, 1090-1097. | 3.1 | 1 |
| 6 | Thermodynamics, Electronic Structure, and Vibrational Properties of Snn(S1â€“xSex)m Solid Solutions for Energy Applications. Chemistry of Materials, 2019, 31, 3672-3685. | 3.2 | 11 |
| 7 | Targeting ideal acceptor-donor materials based on hexabenzocoronene. Journal of Molecular Structure, 2018, 1161, 442-452. | 1.8 | 5 |
| 8 | A combined experimental/theoretical approach to accelerated fuel cell development by quantitative prediction of redox potentials. Journal of Power Sources, 2018, 399, 443-447. | 4.0 | 2 |
| 9 | A perspective on using experiment and theory to identify design principles in dye-sensitized solar cells. Science and Technology of Advanced Materials, 2018, 19, 599-612. | 2.8 | 3 |
| 10 | Monte Carlo simulations of gadolinium doped ceria surfaces. Solid State Ionics, 2018, 324, 128-137. | 1.3 | 8 |
| 11 | 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 |
| 12 | 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 |
| 13 | N<sub>2</sub>O Formation via Reductive Disproportionation of NO by Mononuclear Copper Complexes: A Mechanistic DFT Study. Inorganic Chemistry, 2017, 56, 3820-3833. | 1.9 | 25 |
| 14 | Anab initiocharacterization of the electronic structure of LaCoxFe1-xO3forxâ€‰â‰€â€‰0.5. Physica Status Solidi (B): Basic Research, 2016, 253, 1673-1687. | 0.7 | 0 |
| 15 | 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 |
| 16 | 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 |
| 17 | <scp>C</scp>hem<scp>S</scp>hellâ€”a modular software package for <scp>QM</scp>/<scp>MM</scp> simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 101-110. | 6.2 | 351 |
| 18 | DL_MESO: highly scalable mesoscale simulations. Molecular Simulation, 2013, 39, 796-821. | 0.9 | 123 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Theoretical studies on the reactivity of molybdenum enzymes. Coordination Chemistry Reviews, 2011, 255, 1085-1103. | 9.5 | 50 |
| 20 | 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 |
| 21 | 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 |
| 22 | 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 |
| 23 | 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 |
| 24 | Chloro Complexes with Nitrogen Donors. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2006, 632, 814-818. | 0.6 | 15 |