Dorothea Golze

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3447335/publications.pdf

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21 papers	2,280 citations	623734 14 h-index	713466 21 g-index

21 all docs	21 docs citations	21 times ranked	2310 citing authors

#	Article	IF	Citations
1	CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficient and accurate electronic structure calculations. Journal of Chemical Physics, 2020, 152, 194103.	3.0	1,371
2	The GW Compendium: A Practical Guide to Theoretical Photoemission Spectroscopy. Frontiers in Chemistry, 2019, 7, 377.	3.6	238
3	Toward GW Calculations on Thousands of Atoms. Journal of Physical Chemistry Letters, 2018, 9, 306-312.	4.6	104
4	Importance of dispersion forces for prediction of thermodynamic and transport properties of some common ionic liquids. Physical Chemistry Chemical Physics, 2014, 16, 7209-7221.	2.8	102
5	Core-Level Binding Energies from GW: An Efficient Full-Frequency Approach within a Localized Basis. Journal of Chemical Theory and Computation, 2018, 14, 4856-4869.	5.3	83
6	Simulation of Adsorption Processes at Metallic Interfaces: An Image Charge Augmented QM/MM Approach. Journal of Chemical Theory and Computation, 2013, 9, 5086-5097.	5.3	65
7	Accurate Absolute and Relative Core-Level Binding Energies from GW. Journal of Physical Chemistry Letters, 2020, 11, 1840-1847.	4.6	64
8	Atomic structures and orbital energies of 61,489 crystal-forming organic molecules. Scientific Data, 2020, 7, 58.	5.3	52
9	Wetting of water on hexagonal boron nitride@Rh(111): a QM/MM model based on atomic charges derived for nano-structured substrates. Physical Chemistry Chemical Physics, 2015, 17, 14307-14316.	2.8	42
10	Low-Scaling GW with Benchmark Accuracy and Application to Phosphorene Nanosheets. Journal of Chemical Theory and Computation, 2021, 17, 1662-1677.	5.3	36
11	Accurate Computational Prediction of Core-Electron Binding Energies in Carbon-Based Materials: A Machine-Learning Model Combining Density-Functional Theory and GW. Chemistry of Materials, 2022, 34, 6240-6254.	6.7	22
12	All-Electron BSE@GW Method for K-Edge Core Electron Excitation Energies. Journal of Chemical Theory and Computation, 2022, 18, 1569-1583.	5.3	20
13	Silver-Stabilized Guanine Duplex: Structural and Optical Properties. Journal of Physical Chemistry Letters, 2018, 9, 4789-4794.	4.6	15
14	Relativistic correction scheme for core-level binding energies from GW. Journal of Chemical Physics, 2020, 153, 114110.	3.0	15
15	Quantum embedding theory in the screened Coulomb interaction: Combining configuration interaction with GW/BSE. Physical Review Materials, 2019, 3, .	2.4	14
16	Fast evaluation of solid harmonic Gaussian integrals for local resolution-of-the-identity methods and range-separated hybrid functionals. Journal of Chemical Physics, 2017, 146, 034105.	3.0	12
17	Local Fitting of the Kohnâ€“Sham Density in a Gaussian and Plane Waves Scheme for Large-Scale Density Functional Theory Simulations. Journal of Chemical Theory and Computation, 2017, 13, 2202-2214.	5.3	10
18	Implementation of twoâ€qubit and threeâ€qubit quantum computers using liquidâ€state nuclear magnetic resonance. Concepts in Magnetic Resonance Part A: Bridging Education and Research, 2012, 40A, 25-37.	0.5	5

#	Article	IF	Citations
19	From flat to tilted: gradual interfaces in organic thin film growth. Nanoscale, 2020, 12, 3834-3845.	5.6	4
20	Gold diggers: Altered reconstruction of the gold surface by physisorbed aromatic oligomers. Physical Review Materials, 2019, 3, .	2.4	4
21	Editorial: Many-Body Greenâ€™s Functions and the Bethe-Salpeter Equation in Chemistry: From Single Molecules to Complex Systems. Frontiers in Chemistry, 2022, 10, 866492.	3.6	2