Jan Hermann

List of Publications by Year
in descending order

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23 papers	2,020 citations	687363 13 h-index	677142 22 g-index
25 all docs	25 docs citations	25 times ranked	2733 citing authors

#	Article	IF	Citations
1	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. Journal of Chemical Physics, 2020, 152, 124101.	3.0	589
2	First-Principles Models for van der Waals Interactions in Molecules and Materials: Concepts, Theory, and Applications. Chemical Reviews, 2017, 117, 4714-4758.	47.7	408
3	Recent developments in the P<scp>y</scp>SCF program package. Journal of Chemical Physics, 2020, 153, 024109.	3.0	388
4	Deep-neural-network solution of the electronic SchrÃ¶dinger equation. Nature Chemistry, 2020, 12, 891-897.	13.6	272
5	Nanoscale Ï€â€“Ï€ stacked molecules are bound by collective charge fluctuations. Nature Communications, 2017, 8, 14052.	12.8	69
6	Density Functional Model for van der Waals Interactions: Unifying Many-Body Atomic Approaches with Nonlocal Functionals. Physical Review Letters, 2020, 124, 146401.	7.8	53
7	Theoretical investigation of the FriedlÃnder reaction catalysed by CuBTC: Concerted effect of the adjacent Cu2+ sites. Catalysis Today, 2013, 204, 101-107.	4.4	33
8	Theoretical investigation of layered zeolite frameworks: Surface properties of 2D zeolites. Catalysis Today, 2014, 227, 2-8.	4.4	25
9	Unifying Microscopic and Continuum Treatments of van der Waals and Casimir Interactions. Physical Review Letters, 2017, 118, 266802.	7.8	25
10	Electronic Exchange and Correlation in van der Waals Systems: Balancing Semilocal and Nonlocal Energy Contributions. Journal of Chemical Theory and Computation, 2018, 14, 1361-1369.	5.3	25
11	Coulomb interactions between dipolar quantum fluctuations in van der Waals bound molecules and materials. Nature Communications, 2021, 12, 137.	12.8	21
12	A novel correction scheme for DFT: A combined vdW-DF/CCSD(T) approach. Journal of Chemical Physics, 2013, 139, 034115.	3.0	18
13	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCE<scp>ngine</scp>): Automation and interoperability among computational chemistry programs. Journal of Chemical Physics, 2021, 155, 204801.	3.0	15
14	Phonon-Polariton Mediated Thermal Radiation and Heat Transfer among Molecules and Macroscopic Bodies: Nonlocal Electromagnetic Response at Mesoscopic Scales. Physical Review Letters, 2018, 121, 045901.	7.8	13
15	Convergence to the fixed-node limit in deep variational Monte Carlo. Journal of Chemical Physics, 2021, 154, 124108.	3.0	13
16	Anisotropic Interlayer Force Field for Transition Metal Dichalcogenides: The Case of Molybdenum Disulfide. Journal of Chemical Theory and Computation, 2021, 17, 7237-7245.	5.3	12
17	Communication: Many-body stabilization of non-covalent interactions: Structure, stability, and mechanics of Ag3Co(CN)6 framework. Journal of Chemical Physics, 2016, 145, 241101.	3.0	11
18	Tuning Intermolecular Interactions with Nanostructured Environments. Chemistry of Materials, 2017, 29, 2452-2458.	6.7	9

#	Article	IF	Citations
19	Impact of nuclear vibrations on van der Waals and Casimir interactions at zero and finite temperature. Science Advances, 2019, 5, eaaw0456.	10.3	7
20	Nonlocal Electronic Correlations in the Cohesive Properties of High-Pressure Hydrogen Solids. Journal of Physical Chemistry Letters, 2020, 11, 1521-1527.	4.6	6
21	van der Waals Interactions in Material Modelling. , 2018, , 1-33.		2
22	Fluctuational electrodynamics in atomic and macroscopic systems: van der Waals interactions and radiative heat transfer. Physical Review B, 2020, 102, .	3.2	2
23	Van der Waals Interactions in Material Modelling. , 2020, , 259-291.		0