Jan Hermann

List of Publications by Year
in descending order

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		686830	676716
23	2,020	13	22
papers	citations	h-index	g-index

25	25	25	2733
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Convergence to the fixed-node limit in deep variational Monte Carlo. Journal of Chemical Physics, 2021, 154, 124108.	1.2	13
2	Coulomb interactions between dipolar quantum fluctuations in van der Waals bound molecules and materials. Nature Communications, 2021, 12, 137.	5.8	21
3	Anisotropic Interlayer Force Field for Transition Metal Dichalcogenides: The Case of Molybdenum Disulfide. Journal of Chemical Theory and Computation, 2021, 17, 7237-7245.	2.3	12
4	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.	1.2	15
5	Recent developments in the P<scp>y</scp>SCF program package. Journal of Chemical Physics, 2020, 153, 024109.	1.2	388
6	Fluctuational electrodynamics in atomic and macroscopic systems: van der Waals interactions and radiative heat transfer. Physical Review B, 2020, 102, .	1.1	2
7	Deep-neural-network solution of the electronic SchrÃ¶dinger equation. Nature Chemistry, 2020, 12, 891-897.	6.6	272
8	DFTB+, a software package for efficient approximate density functional theory based atomistic simulations. Journal of Chemical Physics, 2020, 152, 124101.	1.2	589
9	Nonlocal Electronic Correlations in the Cohesive Properties of High-Pressure Hydrogen Solids. Journal of Physical Chemistry Letters, 2020, 11, 1521-1527.	2.1	6
10	Density Functional Model for van der Waals Interactions: Unifying Many-Body Atomic Approaches with Nonlocal Functionals. Physical Review Letters, 2020, 124, 146401.	2.9	53
11	Van der Waals Interactions in Material Modelling. , 2020, , 259-291.		0
12	Impact of nuclear vibrations on van der Waals and Casimir interactions at zero and finite temperature. Science Advances, 2019, 5, eaaw0456.	4.7	7
13	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.	2.3	25
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.	2.9	13
15	van der Waals Interactions in Material Modelling. , 2018, , 1-33.		2
16	First-Principles Models for van der Waals Interactions in Molecules and Materials: Concepts, Theory, and Applications. Chemical Reviews, 2017, 117, 4714-4758.	23.0	408
17	Nanoscale Ï€â€“Ï€ stacked molecules are bound by collective charge fluctuations. Nature Communications, 2017, 8, 14052.	5.8	69
18	Unifying Microscopic and Continuum Treatments of van der Waals and Casimir Interactions. Physical Review Letters, 2017, 118, 266802.	2.9	25

#	Article	IF	Citations
19	Tuning Intermolecular Interactions with Nanostructured Environments. Chemistry of Materials, 2017, 29, 2452-2458.	3.2	9
20	Communication: Many-body stabilization of non-covalent interactions: Structure, stability, and mechanics of Ag3Co(CN)6 framework. Journal of Chemical Physics, 2016, 145, 241101.	1.2	11
21	Theoretical investigation of layered zeolite frameworks: Surface properties of 2D zeolites. Catalysis Today, 2014, 227, 2-8.	2.2	25
22	A novel correction scheme for DFT: A combined vdW-DF/CCSD(T) approach. Journal of Chemical Physics, 2013, 139, 034115.	1.2	18
23	Theoretical investigation of the FriedlÃnder reaction catalysed by CuBTC: Concerted effect of the adjacent Cu2+ sites. Catalysis Today, 2013, 204, 101-107.	2.2	33