Andreas GrÃ¼neis

List of Publications by Year
in descending order

50 papers	3,981 citations	147566 31 h-index	205818 48 g-index
51 all docs	51 docs citations	51 times ranked	3624 citing authors

#	Article	IF	Citations
1	Accurate surface and adsorption energies from many-body perturbation theory. Nature Materials, 2010, 9, 741-744.	13.3	476
2	Towards an exact description of electronic wavefunctions in real solids. Nature, 2013, 493, 365-370.	13.7	440
3	Band alignment of semiconductors from density-functional theory and many-body perturbation theory. Physical Review B, 2014, 90, .	1.1	271
4	Making the random phase approximation to electronic correlation accurate. Journal of Chemical Physics, 2009, 131, 154115.	1.2	227
5	Second-order MÃ¸llerâ€“Plesset perturbation theory applied to extended systems. I. Within the projector-augmented-wave formalism using a plane wave basis set. Journal of Chemical Physics, 2009, 130, 184103.	1.2	194
6	Ionization Potentials of Solids: The Importance of Vertex Corrections. Physical Review Letters, 2014, 112, 096401.	2.9	184
7	Structural and electronic properties of lead chalcogenides from first principles. Physical Review B, 2007, 75, .	1.1	182
8	Second-order MÃ¸llerâ€“Plesset perturbation theory applied to extended systems. II. Structural and energetic properties. Journal of Chemical Physics, 2010, 133, 074107.	1.2	147
9	Assessment of correlation energies based on the random-phase approximation. New Journal of Physics, 2012, 14, 043002.	1.2	137
10	Hybrid functionals including random phase approximation correlation and second-order screened exchange. Journal of Chemical Physics, 2010, 132, 094103.	1.2	131
11	Van der Waals interactions between hydrocarbon molecules and zeolites: Periodic calculations at different levels of theory, from density functional theory to the random phase approximation and MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2012, 137, 114111.	1.2	123
12	Natural Orbitals for Wave Function Based Correlated Calculations Using a Plane Wave Basis Set. Journal of Chemical Theory and Computation, 2011, 7, 2780-2785.	2.3	117
13	Convergence of many-body wave-function expansions using a plane-wave basis: From homogeneous electron gas to solid state systems. Physical Review B, 2012, 86, .	1.1	101
14	Full configuration interaction perspective on the homogeneous electron gas. Physical Review B, 2012, 85, .	1.1	99
15	Physisorption of Water on Graphene: Subchemical Accuracy from Many-Body Electronic Structure Methods. Journal of Physical Chemistry Letters, 2019, 10, 358-368.	2.1	90
16	Applying the Coupled-Cluster Ansatz to Solids and Surfaces in the Thermodynamic Limit. Physical Review X, 2018, 8, .	2.8	80
17	Coupled Cluster Theory in Materials Science. Frontiers in Materials, 2019, 6, .	1.2	74
18	Many-Body Quantum Chemistry for the Electron Gas: Convergent Perturbative Theories. Physical Review Letters, 2013, 110, 226401.	2.9	69

#	Article	IF	Citations
19	Protecting a Diamond Quantum Memory by Charge State Control. Nano Letters, 2017, 17, 5931-5937.	4.5	66
20	Explicitly correlated plane waves: Accelerating convergence in periodic wavefunction expansions. Journal of Chemical Physics, 2013, 139, 084112.	1.2	62
21	Low rank factorization of the Coulomb integrals for periodic coupled cluster theory. Journal of Chemical Physics, 2017, 146, 124105.	1.2	60
22	From plane waves to local Gaussians for the simulation of correlated periodic systems. Journal of Chemical Physics, 2016, 145, 084111.	1.2	56
23	Perspective: Explicitly correlated electronic structure theory for complex systems. Journal of Chemical Physics, 2017, 146, 080901.	1.2	51
24	Surface Floating 2D Bands in Layered Nonsymmorphic Semimetals: ZrSiS and Related Compounds. Physical Review X, 2017, 7, .	2.8	48
25	Communication: Finite size correction in periodic coupled cluster theory calculations of solids. Journal of Chemical Physics, 2016, 145, 141102.	1.2	47
26	Detecting Individual Electrons Using a Carbon Nanotube Field-Effect Transistor. Nano Letters, 2007, 7, 3766-3769.	4.5	44
27	Efficient Explicitly Correlated Many-Electron Perturbation Theory for Solids: Application to the Schottky Defect in MgO. Physical Review Letters, 2015, 115, 066402.	2.9	43
28	Properties of the water to boron nitride interaction: From zero to two dimensions with benchmark accuracy. Journal of Chemical Physics, 2017, 147, 044710.	1.2	43
29	A comparison between quantum chemistry and quantum Monte Carlo techniques for the adsorption of water on the (001) LiH surface. Journal of Chemical Physics, 2017, 146, 204108.	1.2	35
30	A coupled cluster and MÃ¸ller-Plesset perturbation theory study of the pressure induced phase transition in the LiH crystal. Journal of Chemical Physics, 2015, 143, 102817.	1.2	32
31	Ab initio calculations of carbon and boron nitride allotropes and their structural phase transitions using periodic coupled cluster theory. Physical Review B, 2018, 98, .	1.1	28
32	Local embedding of coupled cluster theory into the random phase approximation using plane waves. Journal of Chemical Physics, 2021, 154, 011101.	1.2	24
33	Duality of Ring and Ladder Diagrams and Its Importance for Many-Electron Perturbation Theories. Physical Review Letters, 2019, 123, 156401.	2.9	19
34	A periodic equation-of-motion coupled-cluster implementation applied to F-centers in alkaline earth oxides. Journal of Chemical Physics, 2021, 154, 064106.	1.2	19
35	Screened Exchange Corrections to the Random Phase Approximation from Many-Body Perturbation Theory. Journal of Chemical Theory and Computation, 2019, 15, 3223-3236.	2.3	17
36	A comparative study using state-of-the-art electronic structure theories on solid hydrogen phases under high pressures. Npj Computational Materials, 2019, 5, .	3.5	16

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37	A shortcut to the thermodynamic limit for quantum many-body calculations of metals. Nature Computational Science, 2021, 1, 801-808.	3.8	14
38	A many-electron perturbation theory study of the hexagonal boron nitride bilayer system*. European Physical Journal B, 2016, 89, 1.	0.6	11
39	Reaction energetics of hydrogen on Si(100) surface: A periodic many-electron theory study. Journal of Chemical Physics, 2018, 149, 244105.	1.2	11
40	Particle-particle ladder based basis-set corrections applied to atoms and molecules using coupled-cluster theory. Journal of Chemical Physics, 2019, 151, 104107.	1.2	11
41	Nonlinear behavior of the band gap of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Pb</mml:mtext></mml:mrow><mml:mrow><mml:mn>1</mml:mn></mml:mrow> xmlns:mml="http://www.w3.org/1998/Math/MathML"		