Andreas Grneis

List of Publications by Citations

46 papers	3,222 citations	30 h-index	51 g-index
51 ext. papers	3,609 ext. citations	6.2 avg, IF	5.58 L-index

#	Paper	IF	Citations
46	Accurate surface and adsorption energies from many-body perturbation theory. *Nature Materials*, **2010**, 9, 741-4	27	414
45	Towards an exact description of electronic wavefunctions in real solids. *Nature*, **2013**, 493, 365-70	50.4	375
44	Band alignment of semiconductors from density-functional theory and many-body perturbation theory. *Physical Review B*, **2014**, 90,	3.3	203
43	Making the random phase approximation to electronic correlation accurate. *Journal of Chemical Physics*, **2009**, 131, 154115	3.9	199
42	Second-order MÖller-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	3.9	167
41	Structural and electronic properties of lead chalcogenides from first principles. *Physical Review B*, **2007**, 75,	3.3	166
40	Ionization potentials of solids: the importance of vertex corrections. *Physical Review Letters*, **2014**, 112, 096401	7.4	148
39	Second-order MÖller-Plesset perturbation theory applied to extended systems. II. Structural and energetic properties. *Journal of Chemical Physics*, **2010**, 133, 074107	3.9	125
38	Hybrid functionals including random phase approximation correlation and second-order screened exchange. *Journal of Chemical Physics*, **2010**, 132, 094103	3.9	117
37	Assessment of correlation energies based on the random-phase approximation. *New Journal of Physics*, **2012**, 14, 043002	2.9	111
36	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 MÖller-Plesset perturbation theory. *Journal of Chemical Physics*, **2012**, 137, 114111	3.9	108
35	Natural Orbitals for Wave Function Based Correlated Calculations Using a Plane Wave Basis Set. *Journal of Chemical Theory and Computation*, **2011**, 7, 2780-5	6.4	95
34	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,	3.3	87
33	Full configuration interaction perspective on the homogeneous electron gas. *Physical Review B*, **2012**, 85,	3.3	86
32	Many-body quantum chemistry for the electron gas: convergent perturbative theories. *Physical Review Letters*, **2013**, 110, 226401	7.4	59
31	Explicitly correlated plane waves: accelerating convergence in periodic wavefunction expansions. *Journal of Chemical Physics*, **2013**, 139, 084112	3.9	55
30	Applying the Coupled-Cluster Ansatz to Solids and Surfaces in the Thermodynamic Limit. *Physical Review X*, **2018**, 8,	9.1	53

29	Protecting a Diamond Quantum Memory by Charge State Control. *Nano Letters*, **2017**, 17, 5931-5937	11.5	51
28	Physisorption of Water on Graphene: Subchemical Accuracy from Many-Body Electronic Structure Methods. *Journal of Physical Chemistry Letters*, **2019**, 10, 358-368	6.4	51
27	Low rank factorization of the Coulomb integrals for periodic coupled cluster theory. *Journal of Chemical Physics*, **2017**, 146, 124105	3.9	47
26	Perspective: Explicitly correlated electronic structure theory for complex systems. *Journal of Chemical Physics*, **2017**, 146, 080901	3.9	45
25	From plane waves to local Gaussians for the simulation of correlated periodic systems. *Journal of Chemical Physics*, **2016**, 145, 084111	3.9	45
24	Detecting Individual Electrons Using a Carbon Nanotube Field-Effect Transistor. *Nano Letters*, **2007**, 7, 3766-3769	11.5	40
23	Efficient Explicitly Correlated Many-Electron Perturbation Theory for Solids: Application to the Schottky Defect in MgO. *Physical Review Letters*, **2015**, 115, 066402	7.4	39
22	Communication: Finite size correction in periodic coupled cluster theory calculations of solids. *Journal of Chemical Physics*, **2016**, 145, 141102	3.9	35
21	Coupled Cluster Theory in Materials Science. *Frontiers in Materials*, **2019**, 6,	4	33
20	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	3.9	31
19	Surface Floating 2D Bands in Layered Nonsymmorphic Semimetals: ZrSiS and Related Compounds. *Physical Review X*, **2017**, 7,	9.1	31
18	Properties of the water to boron nitride interaction: From zero to two dimensions with benchmark accuracy. *Journal of Chemical Physics*, **2017**, 147, 044710	3.9	30
17	A coupled cluster and Møller-Plesset perturbation theory study of the pressure induced phase transition in the LiH crystal. *Journal of Chemical Physics*, **2015**, 143, 102817	3.9	27
16	Ab initio calculations of carbon and boron nitride allotropes and their structural phase transitions using periodic coupled cluster theory. *Physical Review B*, **2018**, 98,	3.3	19
15	Duality of Ring and Ladder Diagrams and Its Importance for Many-Electron Perturbation Theories. *Physical Review Letters*, **2019**, 123, 156401	7.4	14
14	Local embedding of coupled cluster theory into the random phase approximation using plane waves. *Journal of Chemical Physics*, **2021**, 154, 011101	3.9	12
13	Screened Exchange Corrections to the Random Phase Approximation from Many-Body Perturbation Theory. *Journal of Chemical Theory and Computation*, **2019**, 15, 3223-3236	6.4	10
12	Particle-particle ladder based basis-set corrections applied to atoms and molecules using coupled-cluster theory. *Journal of Chemical Physics*, **2019**, 151, 104107	3.9	10

11	A comparative study using state-of-the-art electronic structure theories on solid hydrogen phases under high pressures. *Npj Computational Materials*, **2019**, 5,	10.9	10
10	A many-electron perturbation theory study of the hexagonal boron nitride bilayer system*. *European Physical Journal B*, **2016**, 89, 1	1.2	9
9	Nonlinear behavior of the band gap of Pb1−xEuxSe (0≤x≤1) from first principles. *Physical Review B*, **2008**, 78,	3.3	9
8	A periodic equation-of-motion coupled-cluster implementation applied to F-centers in alkaline earth oxides. *Journal of Chemical Physics*, **2021**, 154, 064106	3.9	7
7	Reaction energetics of hydrogen on Si(100) surface: A periodic many-electron theory study. *Journal of Chemical Physics*, **2018**, 149, 244105	3.9	6
6	Many-electron calculations of the phase stability of ZrO2 polymorphs. *Physical Review Research*, **2020**, 2,	3.9	4
5	Focal-point approach with pair-specific cusp correction for coupled-cluster theory. *Journal of Chemical Physics*, **2021**, 154, 234103	3.9	2
4	Surface science using coupled cluster theory via local Wannier functions and in-RPA-embedding: The case of water on graphitic carbon nitride.. *Journal of Chemical Physics*, **2021**, 155, 244103	3.9	2
3	Coupled Cluster and Quantum Chemistry Schemes for Solids **2020**, 453-468		1
2	A shortcut to the thermodynamic limit for quantum many-body calculations of metals. *Nature Computational Science*, **2021**, 1, 801-808		1
1	Coupled Cluster and Quantum Chemistry Schemes for Solids **2018**, 1-16		