

Andreas Grneis

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Focal-point approach with pair-specific cusp correction for coupled-cluster theory. <i>Journal of Chemical Physics</i> , 2021 , 154, 234103	3.9	2
45	Local embedding of coupled cluster theory into the random phase approximation using plane waves. <i>Journal of Chemical Physics</i> , 2021 , 154, 011101	3.9	12
44	A periodic equation-of-motion coupled-cluster implementation applied to F-centers in alkaline earth oxides. <i>Journal of Chemical Physics</i> , 2021 , 154, 064106	3.9	7
43	Surface science using coupled cluster theory via local Wannier functions and in-RPA-embedding: The case of water on graphitic carbon nitride.. <i>Journal of Chemical Physics</i> , 2021 , 155, 244103	3.9	2
42	A shortcut to the thermodynamic limit for quantum many-body calculations of metals. <i>Nature Computational Science</i> , 2021 , 1, 801-808		1
41	Many-electron calculations of the phase stability of ZrO ₂ polymorphs. <i>Physical Review Research</i> , 2020 , 2,	3.9	4
40	Coupled Cluster and Quantum Chemistry Schemes for Solids 2020 , 453-468		1
39	Duality of Ring and Ladder Diagrams and Its Importance for Many-Electron Perturbation Theories. <i>Physical Review Letters</i> , 2019 , 123, 156401	7.4	14
38	Coupled Cluster Theory in Materials Science. <i>Frontiers in Materials</i> , 2019 , 6,	4	33
37	Screened Exchange Corrections to the Random Phase Approximation from Many-Body Perturbation Theory. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 3223-3236	6.4	10
36	Particle-particle ladder based basis-set corrections applied to atoms and molecules using coupled-cluster theory. <i>Journal of Chemical Physics</i> , 2019 , 151, 104107	3.9	10
35	A comparative study using state-of-the-art electronic structure theories on solid hydrogen phases under high pressures. <i>Npj Computational Materials</i> , 2019 , 5,	10.9	10
34	Physisorption of Water on Graphene: Subchemical Accuracy from Many-Body Electronic Structure Methods. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 358-368	6.4	51
33	Reaction energetics of hydrogen on Si(100) surface: A periodic many-electron theory study. <i>Journal of Chemical Physics</i> , 2018 , 149, 244105	3.9	6
32	Ab initio calculations of carbon and boron nitride allotropes and their structural phase transitions using periodic coupled cluster theory. <i>Physical Review B</i> , 2018 , 98,	3.3	19
31	Coupled Cluster and Quantum Chemistry Schemes for Solids 2018 , 1-16		
30	Applying the Coupled-Cluster Ansatz to Solids and Surfaces in the Thermodynamic Limit. <i>Physical Review X</i> , 2018 , 8,	9.1	53

29	Low rank factorization of the Coulomb integrals for periodic coupled cluster theory. <i>Journal of Chemical Physics</i> , 2017 , 146, 124105	3.9	47
28	A comparison between quantum chemistry and quantum Monte Carlo techniques for the adsorption of water on the (001) LiH surface. <i>Journal of Chemical Physics</i> , 2017 , 146, 204108	3.9	31
27	Perspective: Explicitly correlated electronic structure theory for complex systems. <i>Journal of Chemical Physics</i> , 2017 , 146, 080901	3.9	45
26	Protecting a Diamond Quantum Memory by Charge State Control. <i>Nano Letters</i> , 2017 , 17, 5931-5937	11.5	51
25	Properties of the water to boron nitride interaction: From zero to two dimensions with benchmark accuracy. <i>Journal of Chemical Physics</i> , 2017 , 147, 044710	3.9	30
24	Surface Floating 2D Bands in Layered Nonsymmorphic Semimetals: ZrSiS and Related Compounds. <i>Physical Review X</i> , 2017 , 7,	9.1	31
23	A many-electron perturbation theory study of the hexagonal boron nitride bilayer system*. <i>European Physical Journal B</i> , 2016 , 89, 1	1.2	9
22	From plane waves to local Gaussians for the simulation of correlated periodic systems. <i>Journal of Chemical Physics</i> , 2016 , 145, 084111	3.9	45
21	Communication: Finite size correction in periodic coupled cluster theory calculations of solids. <i>Journal of Chemical Physics</i> , 2016 , 145, 141102	3.9	35
20	Efficient Explicitly Correlated Many-Electron Perturbation Theory for Solids: Application to the Schottky Defect in MgO. <i>Physical Review Letters</i> , 2015 , 115, 066402	7.4	39
19	A coupled cluster and Møller-Plesset perturbation theory study of the pressure induced phase transition in the LiH crystal. <i>Journal of Chemical Physics</i> , 2015 , 143, 102817	3.9	27
18	Band alignment of semiconductors from density-functional theory and many-body perturbation theory. <i>Physical Review B</i> , 2014 , 90,	3.3	203
17	Ionization potentials of solids: the importance of vertex corrections. <i>Physical Review Letters</i> , 2014 , 112, 096401	7.4	148
16	Explicitly correlated plane waves: accelerating convergence in periodic wavefunction expansions. <i>Journal of Chemical Physics</i> , 2013 , 139, 084112	3.9	55
15	Towards an exact description of electronic wavefunctions in real solids. <i>Nature</i> , 2013 , 493, 365-70	50.4	375
14	Many-body quantum chemistry for the electron gas: convergent perturbative theories. <i>Physical Review Letters</i> , 2013 , 110, 226401	7.4	59
13	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 Møller-Plesset perturbation theory. <i>Journal of Chemical Physics</i> , 2012 , 137, 114111	3.9	108
12	Convergence of many-body wave-function expansions using a plane-wave basis: From homogeneous electron gas to solid state systems. <i>Physical Review B</i> , 2012 , 86,	3.3	87

11	Assessment of correlation energies based on the random-phase approximation. <i>New Journal of Physics</i> , 2012 , 14, 043002	2.9	111
10	Full configuration interaction perspective on the homogeneous electron gas. <i>Physical Review B</i> , 2012 , 85,	3.3	86
9	Natural Orbitals for Wave Function Based Correlated Calculations Using a Plane Wave Basis Set. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 2780-5	6.4	95
8	Accurate surface and adsorption energies from many-body perturbation theory. <i>Nature Materials</i> , 2010 , 9, 741-4	27	414
7	Hybrid functionals including random phase approximation correlation and second-order screened exchange. <i>Journal of Chemical Physics</i> , 2010 , 132, 094103	3.9	117
6	Second-order Møller-Plesset perturbation theory applied to extended systems. II. Structural and energetic properties. <i>Journal of Chemical Physics</i> , 2010 , 133, 074107	3.9	125
5	Making the random phase approximation to electronic correlation accurate. <i>Journal of Chemical Physics</i> , 2009 , 131, 154115	3.9	199
4	Second-order Møller-Plesset perturbation theory applied to extended systems. I. Within the projector-augmented-wave formalism using a plane wave basis set. <i>Journal of Chemical Physics</i> , 2009 , 130, 184103	3.9	167
3	Nonlinear behavior of the band gap of Pb _{1-x} EuxSe (0 ≤ x ≤ 1) from first principles. <i>Physical Review B</i> , 2008 , 78,	3.3	9
2	Structural and electronic properties of lead chalcogenides from first principles. <i>Physical Review B</i> , 2007 , 75,	3.3	166
1	Detecting Individual Electrons Using a Carbon Nanotube Field-Effect Transistor. <i>Nano Letters</i> , 2007 , 7, 3766-3769	11.5	40