

Andreas GrÃ¼neis

List of Publications by Year in descending order

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Version: 2024-02-01

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	Coupled cluster theory for the ground and excited states of two-dimensional quantum dots. Physical Review B, 2022, 105, .	1.1	1
2	Interface to high-performance periodic coupled-cluster theory calculations with atom-centered, localized basis functions. Journal of Open Source Software, 2022, 7, 4040.	2.0	0
3	Local embedding of coupled cluster theory into the random phase approximation using plane waves. Journal of Chemical Physics, 2021, 154, 011101.	1.2	24
4	Structural and electronic properties of solid molecular hydrogen from many-electron theories. Physical Review B, 2021, 103, .	1.1	3
5	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
6	Driven electronic bridge processes via defect states in Th -doped crystals. Physical Review A, 2021, 103, .	1.0	5
7	Focal-point approach with pair-specific cusp correction for coupled-cluster theory. Journal of Chemical Physics, 2021, 154, 234103.	1.2	8
8	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.	1.2	9
9	A shortcut to the thermodynamic limit for quantum many-body calculations of metals. Nature Computational Science, 2021, 1, 801-808.	3.8	14
10	Coupled Cluster and Quantum Chemistry Schemes for Solids. , 2020, , 453-468.		1
11	Many-electron calculations of the phase stability of ZrO_2 polymorphs. Physical Review Research, 2020, 2, .		
12	Duality of Ring and Ladder Diagrams and Its Importance for Many-Electron Perturbation Theories. Physical Review Letters, 2019, 123, 156401.	2.9	19
13	Coupled Cluster Theory in Materials Science. Frontiers in Materials, 2019, 6, .	1.2	74
14	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
15	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
16	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
17	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
18	Reaction energetics of hydrogen on Si(100) surface: A periodic many-electron theory study. Journal of Chemical Physics, 2018, 149, 244105.	1.2	11

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19	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, .	1.1	28
20	Coupled Cluster and Quantum Chemistry Schemes for Solids. , 2018, , 1-16.		0
21	Applying the Coupled-Cluster Ansatz to Solids and Surfaces in the Thermodynamic Limit. <i>Physical Review X</i> , 2018, 8, .	2.8	80
22	Low rank factorization of the Coulomb integrals for periodic coupled cluster theory. <i>Journal of Chemical Physics</i> , 2017, 146, 124105.	1.2	60
23	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.	1.2	35
24	Perspective: Explicitly correlated electronic structure theory for complex systems. <i>Journal of Chemical Physics</i> , 2017, 146, 080901.	1.2	51
25	Protecting a Diamond Quantum Memory by Charge State Control. <i>Nano Letters</i> , 2017, 17, 5931-5937.	4.5	66
26	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.	1.2	43
27	Surface Floating 2D Bands in Layered Nonsymmorphic Semimetals: ZrSiS and Related Compounds. <i>Physical Review X</i> , 2017, 7, .	2.8	48
28	From plane waves to local Gaussians for the simulation of correlated periodic systems. <i>Journal of Chemical Physics</i> , 2016, 145, 084111.	1.2	56
29	Communication: Finite size correction in periodic coupled cluster theory calculations of solids. <i>Journal of Chemical Physics</i> , 2016, 145, 141102.	1.2	47
30	A many-electron perturbation theory study of the hexagonal boron nitride bilayer system*. <i>European Physical Journal B</i> , 2016, 89, 1.	0.6	11
31	Efficient Explicitly Correlated Many-Electron Perturbation Theory for Solids: Application to the Schottky Defect in MgO. <i>Physical Review Letters</i> , 2015, 115, 066402.	2.9	43
32	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.	1.2	32
33	Band alignment of semiconductors from density-functional theory and many-body perturbation theory. <i>Physical Review B</i> , 2014, 90, .	1.1	271
34	Ionization Potentials of Solids: The Importance of Vertex Corrections. <i>Physical Review Letters</i> , 2014, 112, 096401.	2.9	184
35	Explicitly correlated plane waves: Accelerating convergence in periodic wavefunction expansions. <i>Journal of Chemical Physics</i> , 2013, 139, 084112.	1.2	62
36	Towards an exact description of electronic wavefunctions in real solids. <i>Nature</i> , 2013, 493, 365-370.	13.7	440

#	ARTICLE	IF	CITATIONS
37	Many-Body Quantum Chemistry for the Electron Gas: Convergent Perturbative Theories. Physical Review Letters, 2013, 110, 226401.	2.9	69
38	Assessment of correlation energies based on the random-phase approximation. New Journal of Physics, 2012, 14, 043002.	1.2	137
39	Full configuration interaction perspective on the homogeneous electron gas. Physical Review B, 2012, 85, .	1.1	99
40	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. Journal of Chemical Physics, 2012, 137, 114111.	1.2	123
41	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
42	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
43	Accurate surface and adsorption energies from many-body perturbation theory. Nature Materials, 2010, 9, 741-744.	13.3	476
44	Hybrid functionals including random phase approximation correlation and second-order screened exchange. Journal of Chemical Physics, 2010, 132, 094103.	1.2	131
45	Second-order Møller-Plesset perturbation theory applied to extended systems. II. Structural and energetic properties. Journal of Chemical Physics, 2010, 133, 074107.	1.2	147
46	Making the random phase approximation to electronic correlation accurate. Journal of Chemical Physics, 2009, 131, 154115.	1.2	227
47	Second-order Møller-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
48	Nonlinear behavior of the band gap of $\text{Pb}_{1-x}\text{Sn}_x$		