Andreas Hermann

List of Publications by Year
in descending order

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98	2,645	159525	214721
papers	citations	30 h-index	47 g-index

107	107	107	2611
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Second group of high-pressure high-temperature lanthanide polyhydride superconductors. Physical Review B, 2020, 102, .	1.1	116
2	High pressure ices. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 745-750.	3.3	92
3	Study of the Structural and Electronic Properties of Neutral and Charged Niobium-Doped Silicon Clusters: Niobium Encapsulated in Silicon Cages. Journal of Physical Chemistry C, 2016, 120, 677-684.	1.5	89
4	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Li</mml:mi><mml:mi mathvariant="normal">Nb</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>ground- and excited-state properties from first-principles calculations. Physical Review B, 2008, 77, .	1.1	86
5	Ground-State Properties of Crystalline Ice from Periodic Hartree-Fock Calculations and a Coupled-Cluster-Based Many-Body Decomposition of the Correlation Energy. Physical Review Letters, 2008, 101, 183005.	2.9	80
6	Convergence of the many-body expansion of interaction potentials: From van der Waals to covalent and metallic systems. Physical Review A, 2007, 76, .	1.0	74
7	Insights into the geometries, electronic and magnetic properties of neutral and charged palladium clusters. Scientific Reports, 2016, 6, 19656.	1.6	73
8	Evolution of the Structural and Electronic Properties of Medium-Sized Sodium Clusters: A Honeycomb-Like Na₂₀ Cluster. Inorganic Chemistry, 2017, 56, 1241-1248.	1.9	72
9	Deciphering the Structural Evolution and Electronic Properties of Magnesium Clusters: An Aromatic Homonuclear Metal Mg₁₇ Cluster. Journal of Physical Chemistry A, 2016, 120, 7947-7954.	1.1	68
10	Organic molecule adsorption on solid surfaces: chemical bonding, mutual polarisation and dispersion interaction. Applied Physics A: Materials Science and Processing, 2006, 85, 387-397.	1.1	65
11	Convergence of the MÃ¸ller-Plesset perturbation series for the fcc lattices of neon and argon. Physical Review B, 2010, 82, .	1.1	65
12	Strongly bonded water monomers on the ice Ih basal plane: Density-functional calculations. Physical Review B, 2006, 74, .	1.1	64
13	Resolving the Optical Spectrum of Water: Coordination and Electrostatic Effects. Physical Review Letters, 2008, 100, 207403.	2.9	62
14	Spin-orbit effects in structural and electronic properties for the solid state of the group-14 elements from carbon to superheavy element 114. Physical Review B, 2010, 82, .	1.1	61
15	Phase stability and superconductivity of lead hydrides at high pressure. Physical Review B, 2021, 103, .	1.1	60
16	Reactivity ofÂHe withÂionic compounds under high pressure. Nature Communications, 2018, 9, 951.	5.8	59
17	From Wadeâ€“Mingos to Zintlâ€“Klemm at 100 GPa: Binary Compounds of Boron and Lithium. Journal of the American Chemical Society, 2012, 134, 18606-18618.	6.6	56
18	Equation of state for solid neon from quantum theory. Physical Review B, 2009, 80, .	1.1	55

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19	Xenon Suboxides Stable under Pressure. Journal of Physical Chemistry Letters, 2014, 5, 4336-4342.	2.1	49
20	Probing the structural evolution of ruthenium doped germanium clusters: Photoelectron spectroscopy and density functional theory calculations. Scientific Reports, 2016, 6, 30116.	1.6	45
21	Probing the structural and electronic properties of zirconium doped boron clusters: Zr distorted B₁₂ ligand framework. Physical Chemistry Chemical Physics, 2018, 20, 23740-23746.	1.3	43
22	Prediction of Stable Ruthenium Silicides from First-Principles Calculations: Stoichiometries, Crystal Structures, and Physical Properties. ACS Applied Materials & Interfaces, 2015, 7, 26776-26782.	4.0	42
23	The Search for the Species with the Highest Coordination Number. Angewandte Chemie - International Edition, 2007, 46, 2444-2447.	7.2	38
24	Condensed Astatine: Monatomic and Metallic. Physical Review Letters, 2013, 111, 116404.	2.9	38
25	High-pressure phase of brucite stable at Earthâ€™s mantle transition zone and lower mantle conditions. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 13971-13976.	3.3	35
26	Stabilization of ammonia-rich hydrate inside icy planets. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 9003-9008.	3.3	35
27	Stable Lithium Argon compounds under high pressure. Scientific Reports, 2015, 5, 16675.	1.6	34
28	A Chiral Gasâ€“Hydrate Structure Common to the Carbon Dioxideâ€“Water and Hydrogenâ€“Water Systems. Journal of Physical Chemistry Letters, 2017, 8, 4295-4299.	2.1	34
29	Coexistence of plastic and partially diffusive phases in a helium-methane compound. National Science Review, 2020, 7, 1540-1547.	4.6	33
30	Inelastic x-ray investigation of the ferroelectric transition in SnTe. Physical Review B, 2017, 95, .	1.1	32
31	Blueshifting the Onset of Optical UV Absorption for Water under Pressure. Physical Review Letters, 2011, 106, 187403.	2.9	30
32	Computational phase diagrams of noble gas hydrates under pressure. Journal of Chemical Physics, 2015, 143, 154507.	1.2	30
33	Direct Reaction between Copper and Nitrogen at High Pressures and Temperatures. Journal of Physical Chemistry Letters, 2019, 10, 1109-1114.	2.1	30
34	Complete basis set limit second-order MÃ¸llerâ€“Plesset calculations for the fcc lattices of neon, argon, krypton, and xenon. Journal of Chemical Physics, 2009, 131, 244508.	1.2	29
35	Plastic and Superionic Helium Ammonia Compounds under High Pressure and High Temperature. Physical Review X, 2020, 10, .	2.8	28
36	Binary Compounds of Boron and Beryllium: A Rich Structural Arena with Space for Predictions. Chemistry - A European Journal, 2013, 19, 4184-4197.	1.7	26

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37	Exotic Hydrogen Bonding in Compressed Ammonia Hydrides. Journal of Physical Chemistry Letters, 2019, 10, 2761-2766.	2.1	25
38	Phenanthrenequinone Adsorbed on Si(001):Â Geometries, Electronic Properties, and Optical Response. Journal of Physical Chemistry B, 2005, 109, 7928-7933.	1.2	24
39	The Unusual Solid-State Structure of Mercury Oxide: Relativistic Density Functional Calculations for the Group 12 Oxides ZnO, CdO, and HgO. Journal of Physical Chemistry A, 2009, 113, 12427-12432.	1.1	24
40	AuO: Evolving from Dis- to Comproportionation and Back Again. Inorganic Chemistry, 2016, 55, 1278-1286.	1.9	24
41	Probing the Interactions of O₂ with Small Gold Cluster Au_n^Q (n = 2â€“10, Q = 0, â^'1): A Neutral Chemisorbed Complex Au₅O₂ Cluster Predicted. Journal of Physical Chemistry C, 2017, 121, 24886-24893.	1.5	24
42	Mechanical properties of tantalum carbide from high-pressure/high-temperature synthesis and first-principles calculations. Physical Chemistry Chemical Physics, 2020, 22, 5018-5023.	1.3	24
43	LiB and its boron-deficient variants under pressure. Physical Review B, 2012, 86, .	1.1	23
44	Ternary Mg-Nb-H polyhydrides under high pressure. Physical Review B, 2021, 104, .	1.1	23
45	Novel phases in ammonia-water mixtures under pressure. Journal of Chemical Physics, 2018, 149, 234501.	1.2	22
46	Optical response ofÏ€-conjugated molecular monolayer adsorbed on the semiconductor Si(001) surface: A first-principles study. Physical Review B, 2005, 71, .	1.1	21
47	Praseodymium polyhydrides synthesized at high temperatures and pressures. Physical Review B, 2019, 100, .	1.1	21
48	The Elusive Structure of CrCl₂â€"A Combined Computational and Gasâ€Phase Electronâ€Ðiffraction Study. Chemistry - A European Journal, 2008, 14, 5130-5143.	1.7	20
49	Making Sense of Boron-Rich Binary Beâ€“B Phases. Inorganic Chemistry, 2012, 51, 9066-9075.	1.9	20
50	Lithium hydroxide, LiOH, at elevated densities. Journal of Chemical Physics, 2014, 141, 024505.	1.2	20
51	Structural and electronic properties of the alkali metal incommensurate phases. Physical Review Materials, 2018, 2, .	0.9	20
52	On the chain-melted phase of matter. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 10297-10302.	3.3	19
53	High Pressure Hydrocarbons Revisited: From van der Waals Compounds to Diamond. Geosciences (Switzerland), 2019, 9, 227.	1.0	18
54	Plastic and superionic phases in ammoniaâ€“water mixtures at high pressures and temperatures. Journal of Physics Condensed Matter, 2020, 32, 184004.	0.7	18

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55	Short range order at the amorphous TiO2â€“water interface probed by silicic acid adsorption and interfacial oligomerization: An ATR-IR and 29Si MAS-NMR study. Journal of Colloid and Interface Science, 2012, 368, 447-455.	5.0	16
56	Prediction of Novel High-Pressure Structures of Magnesium Niobium Dihydride. ACS Applied Materials & Interfaces, 2017, 9, 26169-26176.	4.0	16
57	Free electron to electride transition in dense liquid potassium. Nature Physics, 2021, 17, 955-960.	6.5	15
58	Density functional study ofÎ±â^'CrCl2: Structural, electronic, and magnetic properties. Physical Review B, 2006, 74, .	1.1	14
59	LiBeB: A predicted phase with structural and electronic peculiarities. Physical Review B, 2012, 86, .	1.1	14
60	Isotopic differentiation and sublattice melting in dense dynamic ice. Physical Review B, 2013, 88, .	1.1	14
61	Synthesis of Ni2H3 at high temperatures and pressures. Physical Review B, 2018, 98, .	1.1	14
62	Oxidation- and organic-molecule-induced changes of the Si surface optical anisotropy:ab initiopredictions. Journal of Physics Condensed Matter, 2004, 16, S4323-S4334.	0.7	13
63	Monoclinic high-pressure polymorph of AlOOH predicted from first principles. Physical Review B, 2016, 94, .	1.1	13
64	From small fullerenes to the graphene limit: A harmonic forceâ€field method for fullerenes and a comparison to density functional calculations for <scp>G</scp>oldbergâ€“<scp>C</scp>oxeter fullerenes up to C₉₈₀. Journal of Computational Chemistry, 2016, 37, 10-17.	1.5	12
65	Recovery of metastable dense Bi synthesized by shock compression. Applied Physics Letters, 2019, 114, 120601.	1.5	12
66	Electronically Driven 1D Cooperative Diffusion in a Simple Cubic Crystal. Physical Review X, 2021, 11, .	2.8	12
67	Rules of formation of Hâ€“Câ€“Nâ€“O compounds at high pressure and the fates of planetary ices. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	11
68	Exploration of stable stoichiometries, physical properties and hardness in the Rhâ€“Si system: a first-principles study. RSC Advances, 2015, 5, 53497-53503.	1.7	9
69	High-pressure phase transitions in rubidium and caesium hydroxides. Physical Chemistry Chemical Physics, 2016, 18, 16527-16534.	1.3	9
70	Elasticity of phase-Pi (Al3Si2O7(OH)3) â€“ A hydrous aluminosilicate phase. Physics of the Earth and Planetary Interiors, 2017, 269, 91-97.	0.7	8
71	Ostwald's rule of stages and metastable transitions in the hydrogenâ€“water system at high pressure. Physical Chemistry Chemical Physics, 2018, 20, 26853-26858.	1.3	8
72	On a new nitrogen sX hydrate from ice XVII. Journal of Chemical Physics, 2019, 151, 104305.	1.2	8

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73	Theoretical study of the localization of excess electrons at the surface of ice. Journal of Physics Condensed Matter, 2008, 20, 225003.	0.7	7
74	Pressure-induced localisation of the hydrogen-bond network in KOH-VI. Journal of Chemical Physics, 2015, 143, 244706.	1.2	7
75	Stability of Hydrogen Hydrates from Second-Order MÃ¸llerâ€“Plesset Perturbation Theory. Journal of Physical Chemistry Letters, 2018, 9, 5624-5629.	2.1	7
76	Changes of Fermi surface topology due to the rhombohedral distortion in SnTe. Physical Review B, 2020, 102, .	1.1	7
77	Synthesis of Superconducting Cobalt Trihydride. Journal of Physical Chemistry Letters, 2020, 11, 6420-6425.	2.1	6
78	Adsorption of water on chlorine-terminated Si(111) from first principles: Substrate-induced ordering versus intermolecular interactions. Physical Review B, 2006, 73, .	1.1	5
79	Nucleation of Antiferromagnetically Coupled Chromium Dihalides: from Small Clusters to the Solid State. Inorganic Chemistry, 2010, 49, 3169-3182.	1.9	5
80	The Close Relationships between the Crystal Structures of MO and MSO4(M = Group 10, 11, or 12) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 2013, 2013, 5094-5102.	1.0	5
81	Ionic Phases of Ammonia-Rich Hydrate at High Densities. Physical Review Letters, 2021, 126, 015702.	2.9	5
82	Formation and Stability of Dense Methane-Hydrogen Compounds. Physical Review Letters, 2022, 128, .	2.9	5
83	Ammonium fluorideâ€™s analogy to ice: Possibilities and limitations. Journal of Chemical Physics, 2021, 154, 204501.	1.2	4
84	Superionicity, disorder, and bandgap closure in dense hydrogen chloride. Science Advances, 2021, 7, eabi9507.	4.7	4
85	Recoverable high-energy compounds by reacting methane and nitrogen under high pressure. Physical Review Materials, 2020, 4, .	0.9	4
86	Anomalous elasticity of talc at high pressures: Implications for subduction systems. Geoscience Frontiers, 2022, 13, 101381.	4.3	4
87	Temperature-induced electride transition in dense lithium. Physical Review B, 2022, 105, .	1.1	4
88	Geoscience material structures prediction via CALYPSO methodology. Chinese Physics B, 2019, 28, 106107.	0.7	3
89	Ab initio study of pressure-induced structural and electronic phase transitions in Ca2RuO4. Physical Review B, 2021, 104, .	1.1	3
90	Si(001) surface optical anisotropies induced by Ï€-conjugated overlayers and oxidation. Current Applied Physics, 2006, 6, 525-530.	1.1	2

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91	First-Principles Prediction of Structures and Properties in Crystals. Crystals, 2019, 9, 463.	1.0	2
92	First principles study of dense and metallic nitric sulfur hydrides. Communications Chemistry, 2021, 4, .	2.0	2
93	Two-state model for critical points and the negative slope of the melting curve. Physical Review B, 2021, 104, .	1.1	2
94	Non-Fermi liquid behavior below the NÃ©el temperature in the frustrated heavy fermion magnet UAu ₂. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	2
95	Î±-CrCl₂ under Pressure: Prediction of a Metallic Phase Transition. Journal of Physical Chemistry A, 2009, 113, 12022-12027.	1.1	1
96	New Gas Hydrates at High Pressure. Journal of Physics: Conference Series, 2017, 950, 032010.	0.3	0
97	A Density functional approach to the adsorption of water on chlorine-terminate Si(111). , 2006, , 865-868.		0
98	Ammonia Mono Hydrate IV: An Attempted Structure Solution. Crystals, 2022, 12, 135.	1.0	0