Andreas Hermann

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6688472/publications.pdf

Version: 2024-02-01

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	Ammonia Mono Hydrate IV: An Attempted Structure Solution. Crystals, 2022, 12, 135.	1.0	0
2	Anomalous elasticity of talc at high pressures: Implications for subduction systems. Geoscience Frontiers, 2022, 13, 101381.	4.3	4
3	Formation and Stability of Dense Methane-Hydrogen Compounds. Physical Review Letters, 2022, 128, .	2.9	5
4	Temperature-induced electride transition in dense lithium. Physical Review B, 2022, 105, .	1.1	4
5	Electronically Driven 1D Cooperative Diffusion in a Simple Cubic Crystal. Physical Review X, 2021, 11, .	2.8	12
6	Phase stability and superconductivity of lead hydrides at high pressure. Physical Review B, 2021, 103, .	1.1	60
7	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
8	Free electron to electride transition in dense liquid potassium. Nature Physics, 2021, 17, 955-960.	6.5	15
9	Ammonium fluorideâ€™s analogy to ice: Possibilities and limitations. Journal of Chemical Physics, 2021, 154, 204501.	1.2	4
10	First principles study of dense and metallic nitric sulfur hydrides. Communications Chemistry, 2021, 4, .	2.0	2
11	Two-state model for critical points and the negative slope of the melting curve. Physical Review B, 2021, 104, .	1.1	2
12	Ab initio study of pressure-induced structural and electronic phase transitions in Ca2RuO4. Physical Review B, 2021, 104, .	1.1	3
13	Superionicity, disorder, and bandgap closure in dense hydrogen chloride. Science Advances, 2021, 7, eabi9507.	4.7	4
14	Ionic Phases of Ammonia-Rich Hydrate at High Densities. Physical Review Letters, 2021, 126, 015702.	2.9	5
15	Ternary Mg-Nb-H polyhydrides under high pressure. Physical Review B, 2021, 104, .	1.1	23
16	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
17	Synthesis of Superconducting Cobalt Trihydride. Journal of Physical Chemistry Letters, 2020, 11, 6420-6425.	2.1	6
18	Second group of high-pressure high-temperature lanthanide polyhydride superconductors. Physical Review B, 2020, 102, .	1.1	116

#	Article	IF	Citations
19	Changes of Fermi surface topology due to the rhombohedral distortion in SnTe. Physical Review B, 2020, 102, .	1.1	7
20	Coexistence of plastic and partially diffusive phases in a helium-methane compound. National Science Review, 2020, 7, 1540-1547.	4.6	33
21	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
22	Plastic and superionic phases in ammoniaâ€“water mixtures at high pressures and temperatures. Journal of Physics Condensed Matter, 2020, 32, 184004.	0.7	18
23	Plastic and Superionic Helium Ammonia Compounds under High Pressure and High Temperature. Physical Review X, 2020, 10, .	2.8	28
24	Recoverable high-energy compounds by reacting methane and nitrogen under high pressure. Physical Review Materials, 2020, 4, .	0.9	4
25	Geoscience material structures prediction via CALYPSO methodology. Chinese Physics B, 2019, 28, 106107.	0.7	3
26	Praseodymium polyhydrides synthesized at high temperatures and pressures. Physical Review B, 2019, 100, .	1.1	21
27	First-Principles Prediction of Structures and Properties in Crystals. Crystals, 2019, 9, 463.	1.0	2
28	On a new nitrogen sX hydrate from ice XVII. Journal of Chemical Physics, 2019, 151, 104305.	1.2	8
29	Exotic Hydrogen Bonding in Compressed Ammonia Hydrides. Journal of Physical Chemistry Letters, 2019, 10, 2761-2766.	2.1	25
30	High Pressure Hydrocarbons Revisited: From van der Waals Compounds to Diamond. Geosciences (Switzerland), 2019, 9, 227.	1.0	18
31	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
32	Recovery of metastable dense Bi synthesized by shock compression. Applied Physics Letters, 2019, 114, 120601.	1.5	12
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	Reactivity ofÂHe withÂionic compounds under high pressure. Nature Communications, 2018, 9, 951.	5.8	59
35	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
36	Novel phases in ammonia-water mixtures under pressure. Journal of Chemical Physics, 2018, 149, 234501.	1.2	22

#	Article	IF	Citations
37	Synthesis of Ni2H3 at high temperatures and pressures. Physical Review B, 2018, 98, .	1.1	14
38	Stability of Hydrogen Hydrates from Second-Order MÃ¸llerâ€“Plesset Perturbation Theory. Journal of Physical Chemistry Letters, 2018, 9, 5624-5629.	2.1	7
39	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
40	Structural and electronic properties of the alkali metal incommensurate phases. Physical Review Materials, 2018, 2, .	0.9	20
41	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
42	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
43	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
44	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
45	Prediction of Novel High-Pressure Structures of Magnesium Niobium Dihydride. ACS Applied Materials & Interfaces, 2017, 9, 26169-26176.	4.0	16
46	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
47	New Gas Hydrates at High Pressure. Journal of Physics: Conference Series, 2017, 950, 032010.	0.3	0
48	Inelastic x-ray investigation of the ferroelectric transition in SnTe. Physical Review B, 2017, 95, .	1.1	32
49	Insights into the geometries, electronic and magnetic properties of neutral and charged palladium clusters. Scientific Reports, 2016, 6, 19656.	1.6	73
50	Probing the structural evolution of ruthenium doped germanium clusters: Photoelectron spectroscopy and density functional theory calculations. Scientific Reports, 2016, 6, 30116.	1.6	45
51	Monoclinic high-pressure polymorph of AlOOH predicted from first principles. Physical Review B, 2016, 94, .	1.1	13
52	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
53	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
54	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

#	Article	IF	Citations
55	High-pressure phase transitions in rubidium and caesium hydroxides. Physical Chemistry Chemical Physics, 2016, 18, 16527-16534.	1.3	9
56	AuO: Evolving from Dis- to Comproportionation and Back Again. Inorganic Chemistry, 2016, 55, 1278-1286.	1.9	24
57	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
58	Pressure-induced localisation of the hydrogen-bond network in KOH-VI. Journal of Chemical Physics, 2015, 143, 244706.	1.2	7
59	Stable Lithium Argon compounds under high pressure. Scientific Reports, 2015, 5, 16675.	1.6	34
60	Computational phase diagrams of noble gas hydrates under pressure. Journal of Chemical Physics, 2015, 143, 154507.	1.2	30
61	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
62	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
63	Xenon Suboxides Stable under Pressure. Journal of Physical Chemistry Letters, 2014, 5, 4336-4342.	2.1	49
64	Lithium hydroxide, LiOH, at elevated densities. Journal of Chemical Physics, 2014, 141, 024505.	1.2	20
65	Condensed Astatine: Monatomic and Metallic. Physical Review Letters, 2013, 111, 116404.	2.9	38
66	Isotopic differentiation and sublattice melting in dense dynamic ice. Physical Review B, 2013, 88, .	1.1	14
67	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
68	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
69	LiB and its boron-deficient variants under pressure. Physical Review B, 2012, 86, .	1.1	23
70	High pressure ices. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 745-750.	3.3	92
71	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
72	LiBeB: A predicted phase with structural and electronic peculiarities. Physical Review B, 2012, 86, .	1.1	14

#	Article	IF	Citations
73	Making Sense of Boron-Rich Binary Beâ€“B Phases. Inorganic Chemistry, 2012, 51, 9066-9075.	1.9	20
74	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
75	Blueshifting the Onset of Optical UV Absorption for Water under Pressure. Physical Review Letters, 2011, 106, 187403.	2.9	30
76	Nucleation of Antiferromagnetically Coupled Chromium Dihalides: from Small Clusters to the Solid State. Inorganic Chemistry, 2010, 49, 3169-3182.	1.9	5
77	Convergence of the MÃ¸ller-Plesset perturbation series for the fcc lattices of neon and argon. Physical Review B, 2010, 82, .	1.1	65
78	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
79	Equation of state for solid neon from quantum theory. Physical Review B, 2009, 80, .	1.1	55
80	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
81	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
82	Î±-CrCl₂ under Pressure: Prediction of a Metallic Phase Transition. Journal of Physical Chemistry A, 2009, 113, 12022-12027.	1.1	1
83	The Elusive Structure of CrCl₂â€”A Combined Computational and Gasâ€Phase Electronâ€Diffraction Study. Chemistry - A European Journal, 2008, 14, 5130-5143.	1.7	20
84	<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
85	Theoretical study of the localization of excess electrons at the surface of ice. Journal of Physics Condensed Matter, 2008, 20, 225003.	0.7	7
86	Resolving the Optical Spectrum of Water: Coordination and Electrostatic Effects. Physical Review Letters, 2008, 100, 207403.	2.9	62
87	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
88	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
89	The Search for the Species with the Highest Coordination Number. Angewandte Chemie - International Edition, 2007, 46, 2444-2447.	7.2	38
90	Si(001) surface optical anisotropies induced by Ï€-conjugated overlayers and oxidation. Current Applied Physics, 2006, 6, 525-530.	1.1	2

#	Article	IF	Citations
91	Strongly bonded water monomers on the ice Ih basal plane: Density-functional calculations. Physical Review B, 2006, 74, .	1.1	64
92	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
93	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
94	Density functional study ofÎ±â^'CrCl2: Structural, electronic, and magnetic properties. Physical Review B, 2006, 74, .	1.1	14
95	A Density functional approach to the adsorption of water on chlorine-terminate Si(111). , 2006, , 865-868.		0
96	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
97	Phenanthrenequinone Adsorbed on Si(001):Â Geometries, Electronic Properties, and Optical Response. Journal of Physical Chemistry B, 2005, 109, 7928-7933.	1.2	24
98	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