J Christian SchÃ¶n

List of Publications by Year
in descending order

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54	1,858	279798	265206
papers	citations	23 h-index	42 g-index

60	60	60	1501
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular dynamics and DFT study of 38-atom coinage metal clusters. Computational Materials Science, 2022, 201, 110908.	3.0	9
2	Energy landscapes of low-dimensional systems â€“ concepts and examples. Frontiers of Nanoscience, 2022, , 279-310.	0.6	1
3	Energy landscapes of pure and doped ZnO: from bulk crystals to nanostructures. Frontiers of Nanoscience, 2022, , 151-193.	0.6	6
4	Examination of possible high-pressure candidates of SnTiO3: The search for novel ferroelectric materials. APL Materials, 2021, 9, 021103.	5.1	5
5	Exploring energy landscapes at the DFTB quantum level using the threshold algorithm: the case of the anionic metal cluster Au$$_{20}^{-}$$. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	3
6	Real and virtual polymorphism of titanium selenide with robust interatomic potentials. Journal of Materials Chemistry A, 2020, 8, 14054-14061.	10.3	8
7	Shortâ€Range Structural Correlations in Amorphous 2D Polymers. ChemPhysChem, 2019, 20, 2340-2347.	2.1	8
8	Polymorphism in carbohydrate self-assembly at surfaces: STM imaging and theoretical modelling of trehalose on Cu(100). RSC Advances, 2019, 9, 35813-35819.	3.6	15
9	Applications of crystal structure prediction â€“ inorganic and network structures: general discussion. Faraday Discussions, 2018, 211, 613-642.	3.2	6
10	ZnO/ZnS (hetero)structures: ab initio investigations of polytypic behavior of mixed ZnO and ZnS compounds. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2018, 74, 628-642.	1.1	25
11	Structure searching methods: general discussion. Faraday Discussions, 2018, 211, 133-180.	3.2	3
12	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. Faraday Discussions, 2018, 211, 325-381.	3.2	7
13	Applications of crystal structure prediction â€“ organic molecular structures: general discussion. Faraday Discussions, 2018, 211, 493-539.	3.2	8
14	Twoâ€dimensional Siliconâ€Carbon Compounds: Structure Prediction and Band Structures. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2017, 643, 1368-1373.	1.2	12
15	The threshold algorithm: Description of the methodology and new developments. Journal of Chemical Physics, 2017, 147, 152713.	3.0	18
16	Theoretical and Experimental Study of Structural Phases in CoMoO₄â€. Crystal Research and Technology, 2017, 52, 1700069.	1.3	20
17	Combining pressure and temperature control in dynamics on energy landscapes. European Physical Journal B, 2017, 90, 1.	1.5	2
18	Tungsten Disilicide (WSi₂): Synthesis, Characterization, and Prediction of New Crystal Structures. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2017, 643, 2088-2094.	1.2	17

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19	Computational studies of stable hexanuclear Cu_lAg_mAu_n(lâ€‰+â€‰mâ€‰+â€‰nâ€‰=â€‰6; clusters. International Journal of Quantum Chemistry, 2016, 116, 1006-1015.	2.0	6
20	A Threshold-Minimization Scheme for Exploring the Energy Landscape of Biomolecules: Application to a Cyclic Peptide and a Disaccharide. Journal of Chemical Theory and Computation, 2016, 12, 2471-2479.	5.3	6
21	Prediction and clarification of structures of (bio)molecules on surfaces. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2016, 71, 351-374.	0.7	14
22	Rate constants, timescales, and free energy barriers. Journal of Non-Equilibrium Thermodynamics, 2016, 41, 13-18.	4.2	13
23	Ab initiocomputation of the transition temperature of the charge density wave transition in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>TiS</mml:mi><mml:msub><mml:mi mathvariant="normal">e</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2015, 92, .	3.2	44
24	Energy Landscape Exploration of Subâ€Nanometre Copperâ€“Silver Clusters. ChemPhysChem, 2015, 16, 1461-1469.	2.1	20
25	Prediction of possible CaMnO₃modifications using anab initiominimization data-mining approach. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2014, 70, 809-819.	1.1	17
26	How can Databases assist with the Prediction of Chemical Compounds?. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2014, 640, 2717-2726.	1.2	18
27	Determination of the energy landscape of Pd12Pt1 using a combined genetic algorithm and threshold energy method. RSC Advances, 2013, 3, 11571.	3.6	12
28	Evolution of order in amorphous-to-crystalline phase transformation of MgF₂. Journal of Applied Crystallography, 2013, 46, 1105-1116.	4.5	39
29	Energy Landscape Investigations Using the Prescribed Path Method in the ZnO System. Journal of Physical Chemistry C, 2012, 116, 16726-16739.	3.1	34
30	Tetrahelix Conformations and Transformation Pathways in Pt1Pd12 Clusters. Journal of Physical Chemistry A, 2012, 116, 5235-5239.	2.5	15
31	Theoretical and Experimental Exploration of the Energy Landscape of the Quasiâ€Binary Cesium Chloride/Lithium Chloride System. Chemistry - A European Journal, 2012, 18, 3559-3565.	3.3	10
32	Sterically Active Electron Pairs in Lead Sulfide? An Investigation of the Electronic and Vibrational Properties of PbS in the Transition Region Between the Rock Salt and the Î±â€Teâ€Type Modifications. Chemistry - A European Journal, 2012, 18, 10929-10936.	3.3	35
33	A Universal Representation of the States of Chemical Matter Including Metastable Configurations in Phase Diagrams. Angewandte Chemie - International Edition, 2012, 51, 132-135.	13.8	37
34	Competitive trapping in complex state spaces. Journal of Physics A: Mathematical and Theoretical, 2011, 44, 075101.	2.1	10
35	Addressing chemical diversity by employing the energy landscape concept. Acta Crystallographica Section A: Foundations and Advances, 2010, 66, 518-534.	0.3	35
36	Predicting solid compounds via global exploration of the energy landscape of solids on theab initiolevel without recourse to experimental information. Physica Status Solidi (B): Basic Research, 2010, 247, 23-39.	1.5	89

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37	Ab initio prediction of low-temperature phase diagrams in the Alâ€“Gaâ€“Inâ€“As system, MAsâ€“Mâ€²As (M, Mâ€² =) Tj ETQq1 1 0.78 Chemical Physics, 2010, 12, 8491.	2.8	18
38	Structural Insights into 19-Atom Pd/Pt Nanoparticles: A Computational Perspective. Journal of Physical Chemistry C, 2009, 113, 15904-15908.	3.1	21
39	Stability of Alkali Metal Halide Polymorphs as a Function of Pressure. Chemistry - an Asian Journal, 2008, 3, 561-572.	3.3	63
40	Possible Existence of Alkali Metal Orthocarbonates at High Pressure. Chemistry - A European Journal, 2007, 13, 7330-7348.	3.3	35
41	The Route to the Structure Determination of Amorphous Solids: A Case Study of the Ceramic Si3B3N7. Angewandte Chemie - International Edition, 2006, 45, 4244-4263.	13.8	38
42	â€œDesignâ€•in Chemical Synthesisâ€”An Illusion?. Angewandte Chemie - International Edition, 2006, 45, 3406-3412.	13.8	107
43	Kinetic Features of Preferential Trapping on Energy Landscapes. Foundations of Physics Letters, 2005, 18, 171-182.	0.6	25
44	Modeling the solâ€“gel synthesis route of amorphous Si3B3N7. Journal of Materials Chemistry, 2005, 15, 1167-1178.	6.7	23
45	Computational Design and Prediction of Interesting Not-Yet-Synthesized Structures of Inorganic Materials by Using Building Unit Concepts. Chemistry - A European Journal, 2002, 8, 4102-4113.	3.3	105
46	Prediction of high pressure phases in the systems Li3N, Na3N, (Li,Na)3N, Li2S and Na2S. Journal of Materials Chemistry, 2001, 11, 69-77.	6.7	55
47	The lid method for exhaustive exploration of metastable states of complex systems. Computer Physics Communications, 1999, 116, 17-27.	7.5	44
48	Properties of the energy landscape of network models for covalent glasses. Journal of Physics A, 1998, 31, 8165-8178.	1.6	28
49	Preferential trapping on energy landscapes in regions containing deep-lying minima: The reason for the success of simulated annealing?. Journal of Physics A, 1997, 30, 2367-2389.	1.6	37
50	Auf dem Weg zur Syntheseplanung in der FestkÃ¶rperchemie: Vorhersage existenzfÃhiger Strukturkandidaten mit Verfahren zur globalen Strukturoptimierung. Angewandte Chemie, 1996, 108, 1358-1377.	2.0	76
51	First Step Towards Planning of Syntheses in Solid-State Chemistry: Determination of Promising Structure Candidates by Global Optimization. Angewandte Chemie International Edition in English, 1996, 35, 1286-1304.	4.4	268
52	Does the Death Knell Toll for the Metallic Bond?. Angewandte Chemie International Edition in English, 1995, 34, 1081-1083.	4.4	14
53	Contact structure in thermodynamic theory. Reports on Mathematical Physics, 1991, 29, 109-121.	0.8	113
54	Statistical approach to the geometric structure of thermodynamics. Physical Review A, 1990, 41, 3156-3160.	2.5	92