Georg K H Madsen

List of Publications by Year
in descending order

89 papers	9,647 citations	76326 40 h-index	53230 85 g-index
90 all docs	90 docs citations	90 times ranked	10750 citing authors

#	Article	IF	Citations
1	A Differentiable Neural-Network Force Field for Ionic Liquids. Journal of Chemical Information and Modeling, 2022, 62, 88-101.	5.4	17
2	Similarity Clustering for Representative Sets of Inorganic Solids for Density Functional Testing. Journal of Chemical Theory and Computation, 2022, 18, 441-447.	5.3	0
3	What is the optimal mGGA exchange functional for solids?. Journal of Chemical Physics, 2022, 157, .	3.0	3
4	Ultrahigh Thermal Conductivity of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î¸</mml:mi></mml:math> -Phase Tantalum Nitride. Physical Review Letters, 2021, 126, 115901.	7.8	46
5	First-principles self-consistent phonon approach to the study of the vibrational properties and structural phase transition of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BaTiO</mml:mi><mml:mn>3</mml:mn></mml:msub>< Physical Review B, 2021, 103, .	3.2	11
6	How dopants limit the ultrahigh thermal conductivity of boron arsenide: a first principles study. Npj Computational Materials, 2021, 7, .	8.7	21
7	Evolutionary computing and machine learning for discovering of low-energy defect configurations. Npj Computational Materials, 2021, 7, .	8.7	24
8	Phosphateâ€Templated Encapsulation of a {Co^{II}₄O₄} Cubane in Germanotungstates as Carbonâ€Free Homogeneous Water Oxidation Photocatalysts. ChemSusChem, 2021, 14, 2529-2536.	6.8	10
9	119Sn and 7Li Solid-State NMR of the Binary Liâ€"Sn Intermetallics: Structural Fingerprinting and Impact on the Isotropic 119Sn Shift via DFT Calculations. Chemistry of Materials, 2021, 33, 3499-3514.	6.7	10
10	Effects of doping substitutions on the thermal conductivity of half-Heusler compounds. Physical Review B, 2021, 103, .	3.2	5
11	Influence of Onion-like Carbonaceous Particles on the Aggregation Process of Hydrocarbons. ACS Omega, 2021, 6, 27898-27904.	3.5	2
12	Combined treatment of phonon scattering by electrons and point defects explains the thermal conductivity reduction in highly-doped Si. Journal of Materials Chemistry A, 2020, 8, 1273-1278.	10.3	30
13	Localized dimers drive strong anharmonicity and low lattice thermal conductivity in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Zn</mml:mi><mml:msub><mml:mi>Se</mml:mi><mm Physical Review B, 2020, 102, .	3.2	17
14	Shortcomings of meta-GGA functionals when describing magnetism. Physical Review B, 2020, 102, .	3.2	27
15	WIEN2k: An APW+lo program for calculating the properties of solids. Journal of Chemical Physics, 2020, 152, 074101.	3.0	1,185
16	Anomalously large lattice thermal conductivity in metallic tungsten carbide and its origin in the electronic structure. Materials Today Physics, 2020, 13, 100214.	6.0	19
17	A comparative first-principles investigation on the defect chemistry of TiO2 anatase. Journal of Chemical Physics, 2020, 152, 044110.	3.0	12
18	Machine-learning Prediction of Infrared Spectra of Interstellar Polycyclic Aromatic Hydrocarbons. Astrophysical Journal, 2020, 902, 100.	4.5	16

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19	Phonon transport across crystal-phase interfaces and twin boundaries in semiconducting nanowires. Nanoscale, 2019, 11, 16007-16016.	5.6	17
20	Phonon Scattering by Dislocations in GaN. ACS Applied Materials & Interfaces, 2019, 11, 8175-8181.	8.0	25
21	Thermoelectric figure of merit and thermal conductivity of type-I clathrate alloy nanowires. MRS Communications, 2019, 9, 370-374.	1.8	9
22	Comparative study of the PBE and SCAN functionals: The particular case of alkali metals. Journal of Chemical Physics, 2019, 150, 164119.	3.0	16
23	Using nanotubes to study the phonon spectrum of two-dimensional materials. Physical Chemistry Chemical Physics, 2019, 21, 5215-5223.	2.8	3
24	Comparing the performance of LDA and GGA functionals in predicting the lattice thermal conductivity of III-V semiconductor materials in the zincblende structure: The cases of AlAs and BAs. Computational Materials Science, 2019, 156, 354-360.	3.0	30
25	Effect of local chemistry and structure on thermal transport in doped GaAs. Physical Review Materials, 2019, 3, .	2.4	9
26	Resonant phonon scattering in semiconductors. Journal of Materials Chemistry C, 2018, 6, 4691-4697.	5.5	17
27	Materials Screening for the Discovery of New Half-Heuslers: Machine Learning versus ab Initio Methods. Journal of Physical Chemistry B, 2018, 122, 625-632.	2.6	78
28	First-principles quantitative prediction of the lattice thermal conductivity in random semiconductor alloys: The role of force-constant disorder. Physical Review B, 2018, 98, .	3.2	36
29	Orbital-free approximations to the kinetic-energy density in exchange-correlation MGGA functionals: Tests on solids. Journal of Chemical Physics, 2018, 149, 144105.	3.0	17
30	Vibrational Properties of Metastable Polymorph Structures by Machine Learning. Journal of Chemical Information and Modeling, 2018, 58, 2460-2466.	5.4	14
31	BoltzTraP2, a program for interpolating band structures and calculating semi-classical transport coefficients. Computer Physics Communications, 2018, 231, 140-145.	7.5	730
32	Influence of point defects on the thermal conductivity in FeSi. Physical Review B, 2018, 97, .	3.2	21
33	Ab initio lattice thermal conductivity of bulk and thin-film Î±-Al2O3. MRS Communications, 2018, 8, 1119-1123.	1.8	17
34	Phonon transport unveils the prevalent point defects in GaN. Physical Review Materials, 2018, 2, .	2.4	22
35	Lattice thermal conductivity of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ti</mml:mi><mml:mi>x</mml:mi></mml:ms alloys calculated from first principles: Key role of nature of phonon modes. Physical Review B, 2017, 95, .	3.2	79
36	Exceptionally Strong Phonon Scattering by B Substitution in Cubic SiC. Physical Review Letters, 2017, 119, 075902.	7.8	68

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37	<i>Ab initio</i> phonon scattering by dislocations. Physical Review B, 2017, 95, .	3.2	49
38	Novel ternary sulfide thermoelectric materials from high throughput transport and defect calculations. Journal of Materials Chemistry A, 2016, 4, 11086-11093.	10.3	32
39	Two-Step Phase Transition in SnSe and the Origins of its High Power Factor from First Principles. Physical Review Letters, 2016, 117, 276601.	7.8	91
40	A novel p-type half-Heusler from high-throughput transport and defect calculations. Journal of Materials Chemistry C, 2016, 4, 11261-11268.	5.5	64
41	Ab initio investigation of the anomalous phonon softening in FeSi. Physical Review B, 2016, 94, .	3.2	10
42	Extrinsic doping of the half-Heusler compounds. Nanotechnology, 2016, 27, 334002.	2.6	23
43	â€œGlass-likeâ€•thermal conductivity gradually induced in thermoelectric Sr8Ga16Ge30 clathrate by off-centered guest atoms. Journal of Applied Physics, 2016, 119, 185102.	2.5	29
44	High thermoelectric performance of tellurium doped paracostibite. Journal of Materials Chemistry C, 2016, 4, 3094-3100.	5.5	29
45	First principles study of thermal conductivity cross-over in nanostructured zinc-chalcogenides. Journal of Applied Physics, 2015, 117, .	2.5	23
46	Theoretical and experimental investigations of the thermoelectric properties of Bi2S3. Journal of Applied Physics, 2015, 117, .	2.5	55
47	Achieving optimum carrier concentrations in p-doped SnS thermoelectrics. Physical Chemistry Chemical Physics, 2015, 17, 9161-9166.	2.8	23
48	Are Binary Copper Sulfides/Selenides Really New and Promising Thermoelectric Materials?. Advanced Energy Materials, 2014, 4, 1301581.	19.5	227
49	Integrated computational materials discovery of silver doped tin sulfide as a thermoelectric material. Physical Chemistry Chemical Physics, 2014, 16, 19894-19899.	2.8	61
50	High-throughput study of the structural stability and thermoelectric properties of transition metal silicides. New Journal of Physics, 2013, 15, 105010.	2.9	56
51	Environmental tight-binding modeling of nickel and cobalt clusters. Journal of Physics Condensed Matter, 2013, 25, 115502.	1.8	13
52	Ab initio Calculations of Intrinsic Point Defects in ZnSb. Chemistry of Materials, 2012, 24, 2111-2116.	6.7	84
53	High throughput density functional investigations of the stability, electronic structure and thermoelectric properties of binary silicides. Physical Chemistry Chemical Physics, 2012, 14, 16197.	2.8	48
54	Tight-binding simulation of transition-metal alloys. Journal of Physics Condensed Matter, 2011, 23, 276004.	1.8	15

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55	Enhanced Thermoelectric Properties in Zinc Antimonides. Chemistry of Materials, 2011, 23, 3907-3914.	6.7	83
56	Self-consistent meta-generalized gradient approximation study of adsorption of aromatic molecules on noble metal surfaces. Journal of Chemical Physics, 2011, 135, 084704.	3.0	38
57	Alkane dimers interaction: A semi-local MGGA functional study. Chemical Physics Letters, 2010, 492, 183-186.	2.6	17
58	DFT + U study of defects in bulk rutile TiO2. Journal of Chemical Physics, 2010, 133, 144708.	3.0	126
59	Treatment of Layered Structures Using a Semilocal meta-GGA Density Functional. Journal of Physical Chemistry Letters, 2010, 1, 515-519.	4.6	55
60	Electronic structure calculations with GPAW: a real-space implementation of the projector augmented-wave method. Journal of Physics Condensed Matter, 2010, 22, 253202.	1.8	1,451
61	Observation of All the Intermediate Steps of a Chemical Reaction on an Oxide Surface by Scanning Tunneling Microscopy. ACS Nano, 2009, 3, 517-526.	14.6	101
62	2Dâˆ'3D Transition for Cationic and Anionic Gold Clusters: A Kinetic Energy Density Functional Study. Journal of the American Chemical Society, 2009, 131, 10605-10609.	13.7	124
63	Effect of subsurface Ti-interstitials on the bonding of small gold clusters on rutile TiO2(110). Journal of Chemical Physics, 2009, 130, 044704.	3.0	42
64	The Role of Interstitial Sites in the Ti <i>3d</i> Defect State in the Band Gap of Titania. Science, 2008, 320, 1755-1759.	12.6	813
65	An exploration of noble metal substitution in germanium based clathrates. , 2007, , .		1
66	Functional form of the generalized gradient approximation for exchange: ThePBEÎ±functional. Physical Review B, 2007, 75, .	3.2	82
67	Colossal Seebeck coefficient in strongly correlated semiconductor FeSb ₂. Europhysics Letters, 2007, 80, 17008.	2.0	224
68	Crystal structure and transport properties of nickel containing germanium clathrates. Physical Review B, 2007, 76, .	3.2	56
69	The Low-Barrier Hydrogen Bond of Deuterated Benzoylacetone Probed by Very Low Temperature Neutron and X-ray Diffraction Studies and Theoretical Calculations. Chemistry - A European Journal, 2007, 13, 5539-5547.	3.3	26
70	Automated Search for New Thermoelectric Materials: The Case of LiZnSb. Journal of the American Chemical Society, 2006, 128, 12140-12146.	13.7	414
71	Evaluation of27Al and51V Electric Field Gradients and the Crystal Structure for Aluminum Orthovanadate (AlVO4) by Density Functional Theory Calculations. Journal of Physical Chemistry B, 2006, 110, 5975-5983.	2.6	34
72	Crystal Structure, Band Structure, and Physical Properties of Ba8Cu6-xGe40+x(0 â‰xâ‰ 0.7). Chemistry of Materials, 2006, 18, 4633-4642.	6.7	67

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73	Electronic structure in FeSb2, FeAs2 and FeSi. , 2006, , .		3
74	Charge order in magnetite. An LDA+ U study. Europhysics Letters, 2005, 69, 777-783.	2.0	237
75	Refinement of Borate Structures from 11B MAS NMR Spectroscopy and Density Functional Theory Calculations of 11B Electric Field Gradients. Journal of Physical Chemistry A, 2005, 109, 1989-1997.	2.5	68
76	Magnetic structure and electric-field gradients of uranium dioxide: Anab initiostudy. Physical Review B, 2004, 69, .	3.2	155
77	The metalâ€"insulator phase transition in mixed potassiumâ€"rubidium electro-sodalites. Acta Crystallographica Section A: Foundations and Advances, 2004, 60, 450-454.	0.3	2
78	Electronic structure and transport in type-I and type-VIII clathrates containing strontium, barium, and europium. Physical Review B, 2003, 68, .	3.2	251
79	Magnesium: Comparison of density functional theory calculations with electron and x-ray diffraction experiments. Journal of Chemical Physics, 2003, 119, 11359-11366.	3.0	44
80	On the existence of non-nuclear maxima in simple metals. Journal of Chemical Physics, 2002, 117, 8030-8035.	3.0	39
81	Efficient linearization of the augmented plane-wave method. Physical Review B, 2001, 64, .	3.2	914
82	Evaluation of the Solid State Dipole Moment and Pyroelectric Coefficient of Phosphangulene by Multipolar Modeling of X-ray Structure Factors. Chemistry - A European Journal, 2000, 6, 1797-1804.	3.3	42
83	F center in sodium electrosodalite as a physical manifestation of a non-nuclear attractor in the electron density. Physical Review B, 1999, 59, 12359-12369.	3.2	57
84	X-ray and neutron diffraction study of benzoylacetone in the temperature range 8â€"300 K: comparison with other cis-enol molecules. Acta Crystallographica Section B: Structural Science, 1999, 55, 767-787.	1.8	30
85	The Structure of Nitromalonamide:Â A Combined Neutron-Diffraction and Computational Study of a Very Short Hydrogen Bond. Journal of Physical Chemistry A, 1999, 103, 8684-8690.	2.5	43
86	Topological Analysis of the Charge Density in Short Intramolecular Oâˆ'HÂ·Â·Â·O Hydrogen Bonds. Very Low Temperature X-ray and Neutron Diffraction Study of Benzoylacetone. Journal of the American Chemical Society, 1998, 120, 10040-10045.	13.7	153
87	Characterization of the Short Strong Hydrogen Bond in Benzoylacetone by ab Initio Calculations and Accurate Diffraction Experiments. Implications for the Electronic Nature of Low-Barrier Hydrogen Bonds in Enzymatic Reactions. Journal of the American Chemical Society, 1998, 120, 12117-12124.	13.7	120
88	On the electronic nature of low-barrier hydrogen bonds in enzymatic reactions. Proceedings of the National Academy of Sciences of the United States of America, 1998, 95, 12799-12802.	7.1	136
89	Accurate firstâ€principles treatment of the highâ€temperature cubic phase of hafnia. Physica Status Solidi - Rapid Research Letters, 0, , .	2.4	4