Sanwu Wang

List of Publications by Year
in descending order

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35 papers	1,304 citations	430874 18 h-index	361022 35 g-index
35 all docs	35 docs citations	35 times ranked	1502 citing authors

#	Article	IF	Citations
1	Phase diagram and mechanical properties of fifteen quaternary high-entropy metal diborides: First-principles calculations and thermodynamics. Journal of Applied Physics, 2022, 131, .	2.5	10
2	Stability and mechanical properties of single-phase quinary high-entropy metal carbides: First-principles theory and thermodynamics. Journal of the European Ceramic Society, 2022, 42, 3089-3098.	5.7	37
3	First-principles study of thermodynamic miscibility, structures, and optical properties of Cs2Sn(X1â^'xYx)6 (X,Yâ€‰=â€‰I, Br, Cl) lead-free perovskite solar cells. Applied Physics Letters, 2021, 118, .	3.3	19
4	Phase stability, mechanical properties and melting points of high-entropy quaternary metal carbides from first-principles. Journal of the European Ceramic Society, 2021, 41, 6267-6274.	5.7	70
5	Phase transitions and superconductivity of iron-based superconductors from first-principles. Physics Letters, Section A: General, Atomic and Solid State Physics, 2020, 384, 126345.	2.1	5
6	Poisoning and competitive adsorption effects during phenol hydrogenation on platinum in water-alcohol mixtures. Applied Catalysis A: General, 2019, 585, 117199.	4.3	12
7	Ab initio calculations for crystalline PEO6:LiPF6 polymer electrolytes. Computational Materials Science, 2019, 160, 173-179.	3.0	11
8	Solvent-mediated charge separation drives alternative hydrogenation path of furanics in liquid water. Nature Catalysis, 2019, 2, 431-436.	34.4	171
9	Hydrogenation of o-Cresol at the Water/Pt(111) Interface. Journal of Physical Chemistry C, 2019, 123, 5378-5384.	3.1	5
10	Effect of hydrogen coverage on hydrogenation of o-cresol on Pt(111). Applied Surface Science, 2018, 443, 575-580.	6.1	11
11	Electronic structures and transition temperatures of high-T cuprate superconductors from first-principles calculations and Landau theory. Journal of Alloys and Compounds, 2018, 764, 869-880.	5.5	11
12	Sequestration of carbon dioxide in coal: Energetics and bonding from first-principles calculations. Computational Materials Science, 2017, 133, 145-151.	3.0	5
13	Diffusion of Lithium Ions in Amorphous and Crystalline Poly(ethylene oxide)3:LiCF3SO3 Polymer Electrolytes. Electrochimica Acta, 2017, 235, 122-128.	5.2	32
14	Compositional phase diagram and microscopic mechanism of Ba_{1â^'x}Ca_xZr_yTi_{1â^'y}O₃relaxor ferroelectrics. Physical Chemistry Chemical Physics, 2017, 19, 22190-22196.	2.8	27
15	Phase stability, electronic structures, and superconductivity properties of the BaPb_{1â^'x}Bi_xO₃ and Ba_{1â^'x}K_xBiO₃ perovskites. Journal of the American Ceramic Society, 2017, 100, 1221-1230.	3.8	29
16	Hydrogenation of o-cresol on platinum catalyst: Catalytic experiments and first-principles calculations. Applied Surface Science, 2017, 393, 212-220.	6.1	23
17	Compositionâ€•and Pressureâ€Induced Relaxor Ferroelectrics: Firstâ€Principles Calculations and Landauâ€Devonshire Theory. Journal of the American Ceramic Society, 2016, 99, 3336-3342.	3.8	17
18	Ab initio calculations of the atomic and electronic structures of crystalline PEO3:LiCF3SO3 electrolytes. Computational Materials Science, 2016, 112, 170-174.	3.0	9

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19	Modeling and simulations of interface properties with firstâ€principles electronic structure computations. Mathematical Methods in the Applied Sciences, 2015, 38, 4495-4501.	2.3	1
20	Ab initio atomistic thermodynamics study on the oxidation mechanism of binary and ternary alloy surfaces. Journal of Chemical Physics, 2015, 142, 064705.	3.0	18
21	Structure, Phase Transition, and Electronic Properties of <scp><scp>K</scp></scp>_{1â^'x}<scp><scp>Na</scp></scp>_x<scp><scp>NbO</scp></scp> Solid Solutions from Firstâ€Principles Theory. Journal of the American Ceramic Society, 2014, 97, 4019-4023.	3.8	25
22	Phase transformations of nano-sized cubic boron nitride to white graphene and white graphite. Applied Physics Letters, 2014, 104, 093104.	3.3	21
23	Bonding, stability, and electronic properties of the BC<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>honeycomb monolayer structure on NbB<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>(0001). Physical Review B, 2013, 88, .	3.2	15
24	Oxidation of the two-phase Nb/Nb5Si3 composite: The role of energetics, thermodynamics, segregation, and interfaces. Journal of Chemical Physics, 2013, 138, 014708.	3.0	17
25	Oxidation mechanism of the intermetallic compound Ti3Al from ab initio thermodynamics. Physical Chemistry Chemical Physics, 2012, 14, 11160.	2.8	26
26	Increase in oxide hole trap density associated with nitrogen incorporation at the SiO2/SiC interface. Journal of Applied Physics, 2008, 103, .	2.5	69
27	Bonding at theSiCâ^'SiO2Interface and the Effects of Nitrogen and Hydrogen. Physical Review Letters, 2007, 98, 026101.	7.8	171
28	Thermal donor formation processes in silicon and the catalytic role of hydrogen. Applied Physics Letters, 2006, 88, 051916.	3.3	35
29	Total Dose Radiation Response of Nitrided and Non-nitrided SiO$_{2}$/4H-SiC MOS Capacitors. IEEE Transactions on Nuclear Science, 2006, 53, 3687-3692.	2.0	36
30	First-principles calculations for the adsorption of water molecules on theCu(100)surface. Physical Review B, 2004, 70, .	3.2	39
31	Dopants adsorbed as single atoms prevent degradation of catalysts. Nature Materials, 2004, 3, 143-146.	27.5	199
32	Ab initio Monte Carlo simulations for finite-temperature properties: application to lithium clusters and bulk liquid lithium. Computational Materials Science, 2004, 29, 145-151.	3.0	16
33	Atomic-Scale Dynamics of the Formation and Dissolution of Carbon Clusters in SiO2. Physical Review Letters, 2001, 86, 5946-5949.	7.8	86
34	Ab initio HF/DFT studies of the chemisorption of hydrogen on the cluster simulated Si(111)-(â^š3 Ã— Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.9	10
35	Ab initio cluster calculations of the chemisorption of hydrogen on the Si(111)â^š3 Ã— â^š3R30Â°-B surface. Surface Science, 1997, 394, 235-249.	1.9	16