Qingfeng Zeng

List of Publications by Year
in descending order

67	1,321	331259	377514
papers	citations	21 h-index	34 g-index

69	69	69	1649
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	First-principles study on predicting the crystal structures, mechanical properties and electronic structures of HfCxN1-x. Journal of the European Ceramic Society, 2021, 41, 3037-3044.	2.8	7
2	Machine learning and a computational fluid dynamic approach to estimate phase composition of chemical vapor deposition boron carbide. Journal of Advanced Ceramics, 2021, 10, 537-550.	8.9	6
3	High-throughput systematic topological generation of low-energy carbon allotropes. Npj Computational Materials, 2021, 7, .	3.5	14
4	Network topological model of reconstructive solid-state transformations. Scientific Reports, 2019, 9, 6007.	1.6	21
5	Vibrational and dielectric properties of AlN: A first-principles study. Ceramics International, 2016, 42, 18828-18832.	2.3	8
6	Diverse Chemistry of Stable Hydronitrogens, and Implications for Planetary and Materials Sciences. Scientific Reports, 2016, 6, 25947.	1.6	27
7	Numerical Analysis of the Microstructure-based Model for Layered Composites via MC and FEM Approaches. Brazilian Journal of Physics, 2016, 46, 87-96.	0.7	2
8	Pressure-driven formation and stabilization of superconductive chromium hydrides. Scientific Reports, 2015, 5, 17764.	1.6	37
9	First-principles study on the structural and electronic properties of clean and atomic oxygen adsorbed ZrC(0 0 1) surface. Computational Materials Science, 2015, 101, 115-119.	1.4	31
10	Thermodynamic study of the chemical vapor deposition in the SiCl3CH3â€“NH3â€“H2 system. Chemical Physics Letters, 2015, 623, 29-36.	1.2	3
11	PCLab â€“ A software with interactive graphical user interface for Monte Carlo and finite element analysis of microstructure-based layered composites. Advances in Engineering Software, 2015, 90, 53-62.	1.8	5
12	Decomposition reaction rate of BCl3â€“CH4â€“H2 in the gas phase. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	4
13	A Novel Phase of Li₁₅Si₄ Synthesized under Pressure. Advanced Energy Materials, 2015, 5, 1500214.	10.2	14
14	Thermodynamic study on the chemical vapor deposition of silicon nitride from the SiCl4â€“NH3â€“H2 system. Computational and Theoretical Chemistry, 2015, 1051, 93-103.	1.1	3
15	Thermodynamic study on the chemical vapor deposition of boron nitride from the BCl3â€“NH3â€“H2 system. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	4
16	Discovering low-permittivity materials: Evolutionary search for MgAl2O4 polymorphs. Applied Physics Letters, 2014, 105, .	1.5	4
17	Exploration of stable compounds, crystal structures, and superconductivity in the Be-H system. AIP Advances, 2014, 4, .	0.6	25
18	Thermodynamics investigation of the gas-phase reactions in the chemical vapor deposition of silicon borides with BCl3â€“SiCl4â€“H2 precursors. Structural Chemistry, 2014, 25, 1369-1384.	1.0	3

#	Article	IF	Citations
19	Evolutionary search for new high-kdielectric materials: methodology and applications to hafnia-based oxides. Acta Crystallographica Section C, Structural Chemistry, 2014, 70, 76-84.	0.2	44
20	Monte Carlo simulation of polycrystalline microstructures and finite element stress analysis. Materials & Design, 2014, 55, 740-746.	5.1	18
21	Microstructure-based multiphysics modeling for semiconductor integration and packaging. Science Bulletin, 2014, 59, 1696-1708.	1.7	2
22	High throughput exploration of ZrxSi1âˆ’xO2 dielectrics by evolutionary first-principles approaches. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 3549-3553.	0.9	7
23	First-principles calculations of the dielectric and vibrational properties of ferroelectric and paraelectric BaAl2O4. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 1867-1870.	0.9	15
24	Prediction of stable hafnium carbides: Stoichiometries, mechanical properties, and electronic structure. Physical Review B, 2013, 88, .	1.1	51
25	Modeling of Pore Structure Evolution Between Bundles of Plain Woven Fabrics During Chemical Vapor Infiltration Process: The Influence of Preform Geometry. Journal of the American Ceramic Society, 2013, 96, 51-61.	1.9	10
26	Prediction of Permeability for Chemical Vapor Infiltration. Journal of the American Ceramic Society, 2013, 96, 2445-2453.	1.9	12
27	NEW REACTION PATHWAYS OF PROPENE + BCl₃ DECOMPOSITION IN CHEMICAL VAPOR DEPOSITION PROCESS. Journal of Theoretical and Computational Chemistry, 2012, 11, 53-85.	1.8	6
28	Effects of microstructure on vacancy and stress distributions in micro joints under current stressing. , 2012, , .		0
29	Decomposition Reaction Rate of BCl₃â€“C₃H₆(propene)â€“H₂ in the Gas Phase. Journal of Physical Chemistry A, 2012, 116, 6955-6966.	1.1	3
30	Reaction paths of BCl3Â+ÂCH4Â+ÂH2 in the chemical vapor deposition process. Structural Chemistry, 2012, 23, 1677-1692.	1.0	5
31	An atomistic scale study on solidification in ultrafine interconnects. , 2012, , .		0
32	Systematic search for low-enthalpy<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>s</mml:mi><mml:msup><mml:mi>p</mml:mi><mml:mn>3</mml:mn></mml:msup></mml:mrow allotropes using evolutionary metadynamics. Physical Review B, 2012, 85, .	1.1	8
33	Initial decomposition of methyltrichlorosilane in the chemical vapor deposition of silicon-carbide. Computational and Theoretical Chemistry, 2011, 967, 265-272.	1.1	5
34	Vibrational and dielectric properties of magnesium aluminate spinel: A first-principles study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2011, 375, 3521-3524.	0.9	21
35	Modeling of pore structure evolution within the fiber bundle during chemical vapor infiltration process. Chemical Engineering Science, 2011, 66, 5852-5861.	1.9	10
36	Thermodynamic Calculation of HfB2 Volatility Diagram. Journal of Phase Equilibria and Diffusion, 2011, 32, 422-427.	0.5	10

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37	Reaction rate of propene pyrolysis. Journal of Computational Chemistry, 2011, 32, 2745-2755.	1.5	5
38	First-principles study of the structural, vibrational, phonon and thermodynamic properties of transition metal carbides TMC (, Zr and Hf). Solid State Communications, 2011, 151, 61-66.	0.9	36
39	Structural, elastic and electronic properties of transition metal carbides TMC (TM=Ti, Zr, Hf and Ta) from first-principles calculations. Solid State Communications, 2011, 151, 602-606.	0.9	92
40	An investigation of the lowest reaction pathway of propeneÂ+ÂBCl3 decomposition in chemical vapor deposition process. Theoretical Chemistry Accounts, 2010, 127, 519-538.	0.5	9
41	The rate-limiting step in the thermal oxidation of silicon carbide. Scripta Materialia, 2010, 62, 654-657.	2.6	12
42	Reaction pathways of propene pyrolysis. Journal of Computational Chemistry, 2010, 31, 1421-1442.	1.5	7
43	First-principles study of the dielectric properties and infrared reflectance spectrum of. Solid State Communications, 2010, 150, 360-363.	0.9	16
44	An ONIOM study of H2O interacting with the C-terminated surface of silicon carbide. Chemical Physics Letters, 2010, 501, 87-92.	1.2	12
45	Surface relaxation and oxygen adsorption behavior of different SiC polytypes: a first-principles study. Journal of Physics Condensed Matter, 2010, 22, 265003.	0.7	22
46	Crystal structure and elastic properties of ZrB compared with ZrB2: A first-principles study. Computational Materials Science, 2010, 49, 814-819.	1.4	79
47	Adsorption of atomic and molecular oxygen on 3C-SiC(111) and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

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55	Preparation and oxidation resistance of 2D C/SiC composites modified by partial boron carbide self-sealing matrix. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2008, 498, 430-436.	2.6	33
56	Investigation of thermodynamic properties of gaseous SiC(XÂ and aÂ) with accurate model chemistry calculations. Physica A: Statistical Mechanics and Its Applications, 2008, 387, 5440-5456.	1.2	14
57	Thermodynamic investigation of the gas-phase reactions in the chemical vapor deposition of boron carbide with BCl3â€“CH4â€“H2 precursors. Computational and Theoretical Chemistry, 2008, 861, 103-116.	1.5	25
58	Theoretical Investigation for the Activeâ€toâ€Passive Transition in the Oxidation of Silicon Carbide. Journal of the American Ceramic Society, 2008, 91, 1665-1673.	1.9	35
59	Modified Wagner model for the active-to-passive transition in the oxidation of Si₃N₄. Journal Physics D: Applied Physics, 2008, 41, 115412.	1.3	1
60	REACTION THERMODYNAMICS IN CHEMICAL VAPOR DEPOSITION OF BORON CARBIDES WITH BCl₃â€“C₃H₆ (PROPENE)-H₂ PRECURSORS. Journal of Theoretical and Computational Chemistry, 2008, 07, 1269-1312.	1.8	12
61	Modeling the effects of reactor wall reaction on isothermal CVI process of C/SiC composites. Computational Materials Science, 2007, 38, 702-706.	1.4	17
62	Gas-phase reaction thermodynamics in preparation of pyrolytic carbon by propylene pyrolysis. Computational Materials Science, 2007, 40, 504-524.	1.4	11
63	Infrared reflectance spectrum of BN calculated from first principles. Solid State Communications, 2007, 141, 262-266.	0.9	106
64	Numerical simulation for fabrication of C/SiC composites in isothermal CVI reactor. Computational Materials Science, 2006, 38, 245-255.	1.4	23
65	Evaluation of the Thermodynamic Data of CH3SiCl3 Based on Quantum Chemistry Calculations. Journal of Physical and Chemical Reference Data, 2006, 35, 1385-1390.	1.9	50
66	First-principles study of vibrational and dielectric properties ofÎ²â˜Si3N4. Physical Review B, 2006, 74, .	1.1	35
67	Designing expert system with artificial neural networks for in situ toughened Si3N4. Materials & Design, 2002, 23, 287-290.	5.1	15