Qingfeng Zeng

List of Publications by Year
in descending order

67 papers	1,321 citations	331670 21 h-index	377865 34 g-index
69 all docs	69 docs citations	69 times ranked	1649 citing authors

#	Article	IF	Citations
1	Infrared reflectance spectrum of BN calculated from first principles. Solid State Communications, 2007, 141, 262-266.	1.9	106
2	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.	1.9	92
3	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></mml:math> allotropes using evolutionary metadynamics. Physical Review B, 2012, 85, .	3.2	82
4	Crystal structure and elastic properties of ZrB compared with ZrB2: A first-principles study. Computational Materials Science, 2010, 49, 814-819.	3.0	79
5	Prediction of stable hafnium carbides: Stoichiometries, mechanical properties, and electronic structure. Physical Review B, 2013, 88, .	3.2	51
6	Evaluation of the Thermodynamic Data of CH3SiCl3 Based on Quantum Chemistry Calculations. Journal of Physical and Chemical Reference Data, 2006, 35, 1385-1390.	4.2	50
7	Evolutionary search for new high-kdielectric materials: methodology and applications to hafnia-based oxides. Acta Crystallographica Section C, Structural Chemistry, 2014, 70, 76-84.	0.5	44
8	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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19	Numerical simulation for fabrication of C/SiC composites in isothermal CVI reactor. Computational Materials Science, 2006, 38, 245-255.	3.0	23
20	Surface relaxation and oxygen adsorption behavior of different SiC polytypes: a first-principles study. Journal of Physics Condensed Matter, 2010, 22, 265003.	1.8	22
21	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.	2.1	21
22	Network topological model of reconstructive solid-state transformations. Scientific Reports, 2019, 9, 6007.	3.3	21
23	Uniform design and regression analysis of LPCVD boron carbide from BCl3â€“CH4â€“H2 system. Applied Surface Science, 2009, 255, 5729-5735.	6.1	20
24	Monte Carlo simulation of polycrystalline microstructures and finite element stress analysis. Materials & Design, 2014, 55, 740-746.	5.1	18
25	Modeling the effects of reactor wall reaction on isothermal CVI process of C/SiC composites. Computational Materials Science, 2007, 38, 702-706.	3.0	17
26	First-principles investigation on initial stage of 2H-SiC(001) surface oxidation. Science Bulletin, 2009, 54, 1487-1494.	9.0	17
27	First-principles study of the dielectric properties and infrared reflectance spectrum of. Solid State Communications, 2010, 150, 360-363.	1.9	16
28	Designing expert system with artificial neural networks for in situ toughened Si3N4. Materials & Design, 2002, 23, 287-290.	5.1	15
29	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.	2.1	15
30	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.	2.6	14
31	A Novel Phase of Li₁₅Si₄ Synthesized under Pressure. Advanced Energy Materials, 2015, 5, 1500214.	19.5	14
32	High-throughput systematic topological generation of low-energy carbon allotropes. Npj Computational Materials, 2021, 7, .	8.7	14
33	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
34	The rate-limiting step in the thermal oxidation of silicon carbide. Scripta Materialia, 2010, 62, 654-657.	5.2	12
35	An ONIOM study of H2O interacting with the C-terminated surface of silicon carbide. Chemical Physics Letters, 2010, 501, 87-92.	2.6	12
36	Prediction of Permeability for Chemical Vapor Infiltration. Journal of the American Ceramic Society, 2013, 96, 2445-2453.	3.8	12

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37	Gas-phase reaction thermodynamics in preparation of pyrolytic carbon by propylene pyrolysis. Computational Materials Science, 2007, 40, 504-524.	3.0	11
38	Modeling of pore structure evolution within the fiber bundle during chemical vapor infiltration process. Chemical Engineering Science, 2011, 66, 5852-5861.	3.8	10
39	Thermodynamic Calculation of HfB2 Volatility Diagram. Journal of Phase Equilibria and Diffusion, 2011, 32, 422-427.	1.4	10
40	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.	3.8	10
41	Designing expert system for in situ toughened Si3N4 based on adaptive neural fuzzy inference system and genetic algorithms. Materials & Design, 2009, 30, 256-259.	5.1	9
42	An investigation of the lowest reaction pathway of propeneÂ+ÂBCl3 decomposition in chemical vapor deposition process. Theoretical Chemistry Accounts, 2010, 127, 519-538.	1.4	9
43	Thermodynamics of the Production of Condensed Phases in the CVD of Methyltrichlorosilane Pyrolysis. Chemical Vapor Deposition, 2009, 15, 281-290.	1.3	8
44	Vibrational and dielectric properties of AlN: A first-principles study. Ceramics International, 2016, 42, 18828-18832.	4.8	8
45	Reaction pathways of propene pyrolysis. Journal of Computational Chemistry, 2010, 31, 1421-1442.	3.3	7
46	High throughput exploration of ZrxSi1â^'xO2 dielectrics by evolutionary first-principles approaches. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 3549-3553.	2.1	7
47	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.	5.7	7
48	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
49	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.	17.4	6
50	Initial decomposition of methyltrichlorosilane in the chemical vapor deposition of silicon-carbide. Computational and Theoretical Chemistry, 2011, 967, 265-272.	2.5	5
51	Reaction rate of propene pyrolysis. Journal of Computational Chemistry, 2011, 32, 2745-2755.	3.3	5
52	Reaction paths of BCl3Â+ÂCH4Â+ÂH2 in the chemical vapor deposition process. Structural Chemistry, 2012, 23, 1677-1692.	2.0	5
53	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.	3.8	5
54	Effect of C/B ratio in reactants on low-pressure CVD boron-doped carbon deposited from a BCl3â€“C3H6â€“H2 mixture. Journal of Coatings Technology Research, 2009, 6, 509-515.	2.5	4

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55	Thermodynamic study on the chemical vapor deposition of boron nitride from the BCl3â€“NH3â€“H2 system. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	4
56	Discovering low-permittivity materials: Evolutionary search for MgAl2O4 polymorphs. Applied Physics Letters, 2014, 105, .	3.3	4
57	Decomposition reaction rate of BCl3â€“CH4â€“H2 in the gas phase. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	4
58	A unified view of materials design: Two-element principle. Materials & Design, 2009, 30, 487-493.	5.1	3
59	Decomposition Reaction Rate of BCl₃â€“C₃H₆(propene)â€“H₂ in the Gas Phase. Journal of Physical Chemistry A, 2012, 116, 6955-6966.	2.5	3
60	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.	2.0	3
61	Thermodynamic study of the chemical vapor deposition in the SiCl3CH3â€“NH3â€“H2 system. Chemical Physics Letters, 2015, 623, 29-36.	2.6	3
62	Thermodynamic study on the chemical vapor deposition of silicon nitride from the SiCl4â€“NH3â€“H2 system. Computational and Theoretical Chemistry, 2015, 1051, 93-103.	2.5	3
63	Microstructure-based multiphysics modeling for semiconductor integration and packaging. Science Bulletin, 2014, 59, 1696-1708.	1.7	2
64	Numerical Analysis of the Microstructure-based Model for Layered Composites via MC and FEM Approaches. Brazilian Journal of Physics, 2016, 46, 87-96.	1.4	2
65	Modified Wagner model for the active-to-passive transition in the oxidation of Si₃N₄. Journal Physics D: Applied Physics, 2008, 41, 115412.	2.8	1
66	Effects of microstructure on vacancy and stress distributions in micro joints under current stressing. , 2012, , .		0
67	An atomistic scale study on solidification in ultrafine interconnects. , 2012, , .		0