

# Qingfeng Zeng

## List of Publications by Year in descending order

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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	First-principles study on predicting the crystal structures, mechanical properties and electronic structures of HfC <sub>x</sub> N <sub>1-x</sub> . Journal of the European Ceramic Society, 2021, 41, 3037-3044.	5.7	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.	17.4	6
3	High-throughput systematic topological generation of low-energy carbon allotropes. Npj Computational Materials, 2021, 7, .	8.7	14
4	Network topological model of reconstructive solid-state transformations. Scientific Reports, 2019, 9, 6007.	3.3	21
5	Vibrational and dielectric properties of AlN: A first-principles study. Ceramics International, 2016, 42, 18828-18832.	4.8	8
6	Diverse Chemistry of Stable Hydronitrogens, and Implications for Planetary and Materials Sciences. Scientific Reports, 2016, 6, 25947.	3.3	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.	1.4	2
8	Pressure-driven formation and stabilization of superconductive chromium hydrides. Scientific Reports, 2015, 5, 17764.	3.3	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.	3.0	31
10	Thermodynamic study of the chemical vapor deposition in the SiCl <sub>3</sub> CH <sub>3</sub> –NH <sub>3</sub> –H <sub>2</sub> system. Chemical Physics Letters, 2015, 623, 29-36.	2.6	3
11	PCLab – 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
12	Decomposition reaction rate of BCl <sub>3</sub> –CH <sub>4</sub> –H <sub>2</sub> in the gas phase. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	4
13	A Novel Phase of Li <sub>15</sub> Si <sub>4</sub> Synthesized under Pressure. Advanced Energy Materials, 2015, 5, 1500214.	19.5	14
14	Thermodynamic study on the chemical vapor deposition of silicon nitride from the SiCl <sub>4</sub> –NH <sub>3</sub> –H <sub>2</sub> system. Computational and Theoretical Chemistry, 2015, 1051, 93-103.	2.5	3
15	Thermodynamic study on the chemical vapor deposition of boron nitride from the BCl <sub>3</sub> –NH <sub>3</sub> –H <sub>2</sub> system. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	4
16	Discovering low-permittivity materials: Evolutionary search for MgAl <sub>2</sub> O <sub>4</sub> polymorphs. Applied Physics Letters, 2014, 105, .	3.3	4
17	Exploration of stable compounds, crystal structures, and superconductivity in the Be-H system. AIP Advances, 2014, 4, .	1.3	25
18	Thermodynamics investigation of the gas-phase reactions in the chemical vapor deposition of silicon borides with BCl <sub>3</sub> –SiCl <sub>4</sub> –H <sub>2</sub> precursors. Structural Chemistry, 2014, 25, 1369-1384.	2.0	3

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19	Evolutionary search for new high- $\kappa$ dielectric materials: methodology and applications to hafnia-based oxides. Acta Crystallographica Section C, Structural Chemistry, 2014, 70, 76-84.	0.5	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 $Zr_xSi_{1-x}O_2$ dielectrics by evolutionary first-principles approaches. Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 3549-3553.	2.1	7
23	First-principles calculations of the dielectric and vibrational properties of ferroelectric and paraelectric $BaAl_2O_4$ . Physics Letters, Section A: General, Atomic and Solid State Physics, 2014, 378, 1867-1870.	2.1	15
24	Prediction of stable hafnium carbides: Stoichiometries, mechanical properties, and electronic structure. Physical Review B, 2013, 88, .	3.2	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.	3.8	10
26	Prediction of Permeability for Chemical Vapor Infiltration. Journal of the American Ceramic Society, 2013, 96, 2445-2453.	3.8	12
27	NEW REACTION PATHWAYS OF $BCl_3$ 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 $BCl_3$ + $C_3H_6$ (propene) + $H_2$ in the Gas Phase. Journal of Physical Chemistry A, 2012, 116, 6955-6966.	2.5	3
30	Reaction paths of $BCl_3 + CH_4 + H_2$ in the chemical vapor deposition process. Structural Chemistry, 2012, 23, 1677-1692.	2.0	5
31	An atomistic scale study on solidification in ultrafine interconnects. , 2012, , .		0
32	Systematic search for low-enthalpy allotropes using evolutionary metadynamics. Physical Review B, 2012, 85, .	2.5	82
33	Initial decomposition of methyltrichlorosilane in the chemical vapor deposition of silicon-carbide. Computational and Theoretical Chemistry, 2011, 967, 265-272.	2.5	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.	2.1	21
35	Modeling of pore structure evolution within the fiber bundle during chemical vapor infiltration process. Chemical Engineering Science, 2011, 66, 5852-5861.	3.8	10
36	Thermodynamic Calculation of $HfB_2$ Volatility Diagram. Journal of Phase Equilibria and Diffusion, 2011, 32, 422-427.	1.4	10

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37	Reaction rate of propene pyrolysis. Journal of Computational Chemistry, 2011, 32, 2745-2755.	3.3	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.	1.9	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.	1.9	92
40	An investigation of the lowest reaction pathway of propene + AlCl <sub>3</sub> decomposition in chemical vapor deposition process. Theoretical Chemistry Accounts, 2010, 127, 519-538.	1.4	9
41	The rate-limiting step in the thermal oxidation of silicon carbide. Scripta Materialia, 2010, 62, 654-657.	5.2	12
42	Reaction pathways of propene pyrolysis. Journal of Computational Chemistry, 2010, 31, 1421-1442.	3.3	7
43	First-principles study of the dielectric properties and infrared reflectance spectrum of. Solid State Communications, 2010, 150, 360-363.	1.9	16
44	An ONIOM study of H <sub>2</sub> O interacting with the C-terminated surface of silicon carbide. Chemical Physics Letters, 2010, 501, 87-92.	2.6	12
45	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
46	Crystal structure and elastic properties of ZrB compared with ZrB <sub>2</sub> : A first-principles study. Computational Materials Science, 2010, 49, 814-819. Adsorption of atomic and molecular oxygen on SiC-SiC(111) and $\text{SiC-SiC}(111)$ xmins:mml="http://www.w3.org/1998/11math/11mathML"	3.0	79
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55	Preparation and oxidation resistance of 2D C/SiC composites modified by partial boron carbide self-sealing matrix. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2008, 498, 430-436.	5.6	33
56	Investigation of thermodynamic properties of gaseous SiC (X <sup>∞</sup> and a <sup>∞</sup> ) with accurate model chemistry calculations. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2008, 387, 5440-5456.	2.6	14
57	Thermodynamic investigation of the gas-phase reactions in the chemical vapor deposition of boron carbide with BCl <sub>3</sub> â€“CH <sub>4</sub> â€“H <sub>2</sub> precursors. <i>Computational and Theoretical Chemistry</i> , 2008, 861, 103-116.	1.5	25
58	Theoretical Investigation for the Activeâ€“toâ€“Passive Transition in the Oxidation of Silicon Carbide. <i>Journal of the American Ceramic Society</i> , 2008, 91, 1665-1673.	3.8	35
59	Modified Wagner model for the active-to-passive transition in the oxidation of Si <sub>3</sub> N <sub>4</sub> . <i>Journal Physics D: Applied Physics</i> , 2008, 41, 115412.	2.8	1
60	REACTION THERMODYNAMICS IN CHEMICAL VAPOR DEPOSITION OF BORON CARBIDES WITH BCl <sub>3</sub> â€“C <sub>3</sub> H <sub>6</sub> (PROPENE)-H <sub>2</sub> PRECURSORS. <i>Journal of Theoretical and Computational Chemistry</i> , 2008, 07, 1269-1312.	1.8	12
61	Modeling the effects of reactor wall reaction on isothermal CVI process of C/SiC composites. <i>Computational Materials Science</i> , 2007, 38, 702-706.	3.0	17
62	Gas-phase reaction thermodynamics in preparation of pyrolytic carbon by propylene pyrolysis. <i>Computational Materials Science</i> , 2007, 40, 504-524.	3.0	11
63	Infrared reflectance spectrum of BN calculated from first principles. <i>Solid State Communications</i> , 2007, 141, 262-266.	1.9	106
64	Numerical simulation for fabrication of C/SiC composites in isothermal CVI reactor. <i>Computational Materials Science</i> , 2006, 38, 245-255.	3.0	23
65	Evaluation of the Thermodynamic Data of CH <sub>3</sub> SiCl <sub>3</sub> Based on Quantum Chemistry Calculations. <i>Journal of Physical and Chemical Reference Data</i> , 2006, 35, 1385-1390.	4.2	50
66	First-principles study of vibrational and dielectric properties of Si <sub>3</sub> N <sub>4</sub> . <i>Physical Review B</i> , 2006, 74, .	3.2	35
67	Designing expert system with artificial neural networks for in situ toughened Si <sub>3</sub> N <sub>4</sub> . <i>Materials &amp; Design</i> , 2002, 23, 287-290.	5.1	15