Rao Huang

List of Publications by Year
in descending order

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58	1,072	394421	454955
papers	citations	19 h-index	30 g-index

58	58	58	1211
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ptâ€“Pd Bimetallic Catalysts: Structural and Thermal Stabilities of Coreâ€“Shell and Alloyed Nanoparticles. Journal of Physical Chemistry C, 2012, 116, 8664-8671.	3.1	104
2	Structure and stability of platinum nanocrystals: from low-index to high-index facets. Journal of Materials Chemistry, 2011, 21, 11578.	6.7	66
3	Synthesis, properties, and optical applications of noble metal nanoparticle-biomolecule conjugates. Science Bulletin, 2012, 57, 238-246.	1.7	64
4	Insight into the Melting Behavior of Auâ€“Pt Coreâ€“Shell Nanoparticles from Atomistic Simulations. Journal of Physical Chemistry C, 2013, 117, 4278-4286.	3.1	62
5	Computational screening of efficient graphene-supported transition metal single atom catalysts toward the oxygen reduction reaction. Journal of Materials Chemistry A, 2020, 8, 19319-19327.	10.3	49
6	Two-Stage Melting in Coreâ€“Shell Nanoparticles: An Atomic-Scale Perspective. Journal of Physical Chemistry C, 2012, 116, 11837-11841.	3.1	48
7	Growth of stoichiometric Cu3N thin films by reactive magnetron sputtering. Journal of Crystal Growth, 2006, 295, 79-83.	1.5	45
8	Enhanced thermal stability of Au@Pt nanoparticles by tuning shell thickness: Insights from atomistic simulations. Journal of Materials Chemistry, 2012, 22, 7380.	6.7	37
9	Tunable thermodynamic stability of Auâ€“CuPt coreâ€“shell trimetallic nanoparticles by controlling the alloy composition: insights from atomistic simulations. Physical Chemistry Chemical Physics, 2014, 16, 22754-22761.	2.8	34
10	Diverse Melting Modes and Structural Collapse of Hollow Bimetallic Core-Shell Nanoparticles: A Perspective from Molecular Dynamics Simulations. Scientific Reports, 2014, 4, 7051.	3.3	34
11	Thermal Stability and Shape Evolution of Tetrahexahedral Auâ€“Pd Coreâ€“Shell Nanoparticles with High-Index Facets. Journal of Physical Chemistry C, 2013, 117, 6896-6903.	3.1	30
12	Mechanical properties of platinum nanowires: An atomistic investigation on single-crystalline and twinned structures. Computational Materials Science, 2012, 55, 205-210.	3.0	25
13	High-index-faceted platinum nanoparticles: insights into structural and thermal stabilities and shape evolution from atomistic simulations. Journal of Materials Chemistry A, 2014, 2, 11480-11489.	10.3	25
14	Single-crystalline and multiple-twinned gold nanoparticles: an atomistic perspective on structural and thermal stabilities. RSC Advances, 2014, 4, 7528.	3.6	25
15	Thermal Stability of Coâ€“Pt and Coâ€“Au Coreâ€“Shell Structured Nanoparticles: Insights from Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2017, 8, 4273-4278.	4.6	23
16	Effect of oxygen inclusion on microstructure and thermal stability of copper nitride thin films. Journal of Materials Research, 2007, 22, 3052-3057.	2.6	22
17	Computational screening of MBene monolayers with high electrocatalytic activity for the nitrogen reduction reaction. Nanoscale, 2021, 13, 15002-15009.	5.6	22
18	Computational screening of pristine and functionalized ordered TiVC MXenes as highly efficient anode materials for lithium-ion batteries. Nanoscale, 2021, 13, 2995-3001.	5.6	22

#	Article	IF	Citations
19	Thermal Stability of Platinumâ€“Cobalt Bimetallic Nanoparticles: Chemically Disordered Alloys, Ordered Intermetallics, and Coreâ€“Shell Structures. ACS Applied Materials & Interfaces, 2017, 9, 12486-12493.	8.0	21
20	Long-time molecular dynamics simulations on massively parallel platforms: A comparison of parallel replica dynamics and parallel trajectory splicing. Journal of Materials Research, 2018, 33, 813-822.	2.6	21
21	Atomic structure and thermal stability of Ptâ€“Fe bimetallic nanoparticles: from alloy to core/shell architectures. Physical Chemistry Chemical Physics, 2016, 18, 17010-17017.	2.8	18
22	Structural and electronic properties of ZnO/GaN heterostructured nanowires from first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 3097-3102.	2.8	18
23	Thermal stability of platinum nanowires: a comparison study between single-crystalline and twinned structures. Journal of Materials Chemistry, 2011, 21, 18998.	6.7	16
24	Tetrahexahedral Ptâ€“Pd alloy nanocatalysts with high-index facets: an atomistic perspective on thermodynamic and shape stabilities. Journal of Materials Chemistry A, 2014, 2, 1375-1382.	10.3	15
25	Single Mn Atom Anchored on Nitrogenâ€Doped Graphene as a Highly Efficient Electrocatalyst for Oxygen Reduction Reaction. Chemistry - A European Journal, 2021, 27, 9686-9693.	3.3	15
26	Cold welding of copper nanowires with single-crystalline and twinned structures: A comparison study. Physica E: Low-Dimensional Systems and Nanostructures, 2016, 83, 329-332.	2.7	13
27	Atomic-scale insights into structural and thermodynamic stability of Pdâ€“Ni bimetallic nanoparticles. Physical Chemistry Chemical Physics, 2016, 18, 9847-9854.	2.8	13
28	Effect of Chemical Ordering on Thermal Stability of Ptâ€“Co Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 12007-12014.	3.1	13
29	Cluster analysis of accelerated molecular dynamics simulations: A case study of the decahedron to icosahedron transition in Pt nanoparticles. Journal of Chemical Physics, 2017, 147, 152717.	3.0	12
30	Basin Hopping Genetic Algorithm for Global Optimization of PtCo Clusters. Journal of Chemical Information and Modeling, 2020, 60, 2219-2228.	5.4	12
31	Direct observations of shape fluctuation in long-time atomistic simulations of metallic nanoclusters. Physical Review Materials, 2018, 2, .	2.4	12
32	Formation of a rosette pattern in copper nitride thin films via nanocrystals gliding. Nanotechnology, 2005, 16, 2092-2095.	2.6	11
33	Boosting the Electrocatalytic Activity of Feâ€'Co Dualâ€Atom Catalysts for Oxygen Reduction Reaction by Ligandâ€Modification Engineering. ChemCatChem, 2021, 13, 4645-4651.	3.7	11
34	Thermal and shape stability of high-index-faceted rhodium nanoparticles: a molecular dynamics investigation. Physical Chemistry Chemical Physics, 2015, 17, 5751-5757.	2.8	10
35	Solidâ€“Liquid Coexistence in Trimetallic Heterostructured Nanoparticle Catalysts: Insights from Molecular Dynamics Simulations. ACS Applied Nano Materials, 2020, 3, 12369-12378.	5.0	10
36	Thermal Stability of Unary to Quinary Noble-Metal/3d-Transition-Metal Alloy Nanoparticles from Molecular Dynamics Simulations: Implications for Multimetallic Catalysis. ACS Applied Nano Materials, 2020, 3, 5381-5389.	5.0	9

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37	Atomic-scale insights into thermal stability of Pt3Co nanoparticles: A comparison between disordered alloy and ordered intermetallics. Journal of Alloys and Compounds, 2019, 776, 629-635.	5.5	9
38	Exploring Highly Efficient Dual-Metal-Site Electrocatalysts for Oxygen Reduction Reaction by First Principles Screening. Journal of the Electrochemical Society, 2022, 169, 026524.	2.9	9
39	Growth of nearly one nanometer large silicon particles in silicon carbide and their quantum-confined photoluminescence features. Nanotechnology, 2007, 18, 445605.	2.6	8
40	Chemically initiated liquid-like behavior and fabrication of periodic wavy Cu/CuAu nanocables with enhanced catalytic properties. Nanoscale, 2018, 10, 9012-9020.	5.6	8
41	Structural Evolution of the Surface and Interface in Bimetallic High-Index Faceted Heterogeneous Nanoparticles. Journal of Physical Chemistry Letters, 2021, 12, 2454-2462.	4.6	5
42	Tunable light emission and decaying process of photoluminescence from a nanostructured Si-in-SiNx film. Journal of Luminescence, 2007, 126, 536-540.	3.1	4
43	Effect of well confinement on photoluminescence features from silicon nanoparticles embedded in an SiC/SiNxmultilayered structure. Nanotechnology, 2008, 19, 255402.	2.6	4
44	Time-resolved photoluminescence from Si-in-SiNx/Si-in-SiC quantum well-dot structures. Optical Materials, 2013, 35, 2414-2417.	3.6	4
45	Octadecahedral and dodecahedral iron nanoparticles: An atomistic simulation on stability and shape evolutions. Physics Letters, Section A: General, Atomic and Solid State Physics, 2016, 380, 739-744.	2.1	4
46	Structural, magnetic, and electronic properties of small M-Pt (MÂ=ÂFe, Co, and Ni) clusters: Insight from density-functional calculations. Journal of Magnetism and Magnetic Materials, 2020, 512, 167047.	2.3	4
47	Oxygen adsorption on high-index faceted Pt nanoparticles. Physical Chemistry Chemical Physics, 2021, 23, 17323-17328.	2.8	4
48	Computational evaluation of ScB and TiB MBenes as promising anode materials for high-performance metal-ion batteries. Physical Review Materials, 2022, 6, .	2.4	4
49	First-Principles Study of Effect of Strain on the Band Structure of ZnO Monolayer. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2015, 31, 1677-1682.	4.9	3
50	Shape Stability of Metallic Nanoplates: A Molecular Dynamics Study. Nanoscale Research Letters, 2019, 14, 357.	5.7	3
51	Structural and magnetic properties of Co-Pt clusters: A spin-polarized density functional study. Journal of Magnetism and Magnetic Materials, 2020, 503, 166651.	2.3	3
52	Molecular Dynamics Simulations of Thermally Induced Surface and Shape Evolution of Concave Au Nanocubes: Implications for Catalysis. ACS Applied Nano Materials, 2021, 4, 9527-9535.	5.0	2
53	Molecular Dynamics Investigation on Thermal Stability and Shape Evolution of Pd-Au Heterostructured Nanorods: Implications for Catalysis. ACS Applied Nano Materials, 0, , .	5.0	2
54	Molecular dynamics investigation of thermal stability of Pt-Au core-shell nanoparticle. Wuli Xuebao/Acta Physica Sinica, 2013, 62, 126101.	0.5	2

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55	An Improved Self-Adaptive Differential Evolution with the Neighborhood Search Algorithm for Global Optimization of Bimetallic Clusters. Journal of Chemical Information and Modeling, 2022, 62, 2398-2408.	5.4	2
56	Thermally activated microstructural evolution of metallic heterophase nanoparticles: insights from molecular dynamics simulations. Nanoscale, 2022, 14, 10236-10244.	5.6	1
57	Synthesis and photoluminescence studies of silicon nanoparticles embedded in silicon compound films. Frontiers of Physics in China, 2008, 3, 173-180.	1.0	0
58	Thermally activated phase transitions in Fe-Ni core-shell nanoparticles. Frontiers of Physics, 2019, 14, 1.	5.0	0