Rao Huang

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/2352890/publications.pdf

Version: 2024-02-01

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	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
2	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
3	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
4	Thermally activated microstructural evolution of metallic heterophase nanoparticles: insights from molecular dynamics simulations. Nanoscale, 2022, 14, 10236-10244.	5.6	1
5	Computational screening of MBene monolayers with high electrocatalytic activity for the nitrogen reduction reaction. Nanoscale, 2021, 13, 15002-15009.	5.6	22
6	Oxygen adsorption on high-index faceted Pt nanoparticles. Physical Chemistry Chemical Physics, 2021, 23, 17323-17328.	2.8	4
7	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
8	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
9	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
10	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
11	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
12	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
13	Basin Hopping Genetic Algorithm for Global Optimization of PtCo Clusters. Journal of Chemical Information and Modeling, 2020, 60, 2219-2228.	5.4	12
14	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
15	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
16	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
17	Solidâ€“Liquid Coexistence in Trimetallic Heterostructured Nanoparticle Catalysts: Insights from Molecular Dynamics Simulations. ACS Applied Nano Materials, 2020, 3, 12369-12378.	5.0	10
18	Thermally activated phase transitions in Fe-Ni core-shell nanoparticles. Frontiers of Physics, 2019, 14, 1.	5.0	0

#	Article	IF	Citations
19	Effect of Chemical Ordering on Thermal Stability of Ptâ€“Co Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 12007-12014.	3.1	13
20	Shape Stability of Metallic Nanoplates: A Molecular Dynamics Study. Nanoscale Research Letters, 2019, 14, 357.	5.7	3
21	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
22	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
23	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
24	Direct observations of shape fluctuation in long-time atomistic simulations of metallic nanoclusters. Physical Review Materials, 2018, 2, .	2.4	12
25	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
26	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
27	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
28	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
29	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
30	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
31	Atomic-scale insights into structural and thermodynamic stability of Pdâ€“Ni bimetallic nanoparticles. Physical Chemistry Chemical Physics, 2016, 18, 9847-9854.	2.8	13
32	Structural and electronic properties of ZnO/GaN heterostructured nanowires from first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 3097-3102.	2.8	18
33	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
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	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
36	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

#	Article	IF	Citations
37	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
38	Single-crystalline and multiple-twinned gold nanoparticles: an atomistic perspective on structural and thermal stabilities. RSC Advances, 2014, 4, 7528.	3.6	25
39	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
40	Time-resolved photoluminescence from Si-in-SiNx/Si-in-SiC quantum well-dot structures. Optical Materials, 2013, 35, 2414-2417.	3.6	4
41	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
42	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
43	Molecular dynamics investigation of thermal stability of Pt-Au core-shell nanoparticle. Wuli Xuebao/Acta Physica Sinica, 2013, 62, 126101.	0.5	2
44	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
45	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
46	Two-Stage Melting in Coreâ€“Shell Nanoparticles: An Atomic-Scale Perspective. Journal of Physical Chemistry C, 2012, 116, 11837-11841.	3.1	48
47	Mechanical properties of platinum nanowires: An atomistic investigation on single-crystalline and twinned structures. Computational Materials Science, 2012, 55, 205-210.	3.0	25
48	Synthesis, properties, and optical applications of noble metal nanoparticle-biomolecule conjugates. Science Bulletin, 2012, 57, 238-246.	1.7	64
49	Structure and stability of platinum nanocrystals: from low-index to high-index facets. Journal of Materials Chemistry, 2011, 21, 11578.	6.7	66
50	Thermal stability of platinum nanowires: a comparison study between single-crystalline and twinned structures. Journal of Materials Chemistry, 2011, 21, 18998.	6.7	16
51	Synthesis and photoluminescence studies of silicon nanoparticles embedded in silicon compound films. Frontiers of Physics in China, 2008, 3, 173-180.	1.0	0
52	Effect of well confinement on photoluminescence features from silicon nanoparticles embedded in an SiC/SiNxmultilayered structure. Nanotechnology, 2008, 19, 255402.	2.6	4
53	Growth of nearly one nanometer large silicon particles in silicon carbide and their quantum-confined photoluminescence features. Nanotechnology, 2007, 18, 445605.	2.6	8
54	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

#	Article	IF	Citations
55	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
56	Growth of stoichiometric Cu3N thin films by reactive magnetron sputtering. Journal of Crystal Growth, 2006, 295, 79-83.	1.5	45
57	Formation of a rosette pattern in copper nitride thin films via nanocrystals gliding. Nanotechnology, 2005, 16, 2092-2095.	2.6	11
58	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