Yu-Hua Wen

List of Publications by Year in Descending Order

104 papers	1,940 citations	24 h-index	39 g-index
109 ext. papers	2,208 ext. citations	4 avg, IF	4.94 L-index

#	Paper	IF	Citations
104	Structural Evolution of the Surface and Interface in Bimetallic High-Index Faceted Heterogeneous Nanoparticles. *Journal of Physical Chemistry Letters*, **2021**, 12, 2454-2462	6.4	5
103	Single Mn Atom Anchored on Nitrogen-Doped Graphene as a Highly Efficient Electrocatalyst for Oxygen Reduction Reaction. *Chemistry - A European Journal*, **2021**, 27, 9686-9693	4.8	2
102	A force sensing structure with orthogonal optical fiber loops for robot fingers. *Optics Communications*, **2021**, 484, 126686	2	0
101	Computational screening of MBene monolayers with high electrocatalytic activity for the nitrogen reduction reaction. *Nanoscale*, **2021**, 13, 15002-15009	7.7	2
100	Oxygen adsorption on high-index faceted Pt nanoparticles. *Physical Chemistry Chemical Physics*, **2021**, 23, 17323-17328	3.6	2
99	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	5.6	0
98	Boosting the Electrocatalytic Activity of Fe□o Dual-Atom Catalysts for Oxygen Reduction Reaction by Ligand-Modification Engineering. *ChemCatChem*, **2021**, 13, 4645	5.2	2
97	Computational screening of pristine and functionalized ordered TiVC MXenes as highly efficient anode materials for lithium-ion batteries. *Nanoscale*, **2021**, 13, 2995-3001	7.7	6
96	Basin Hopping Genetic Algorithm for Global Optimization of PtCo Clusters. *Journal of Chemical Information and Modeling*, **2020**, 60, 2219-2228	6.1	4
95	Structural, magnetic, and electronic properties of small M-Pt (M□=□Fe, Co, and Ni) clusters: Insight from density-functional calculations. *Journal of Magnetism and Magnetic Materials*, **2020**, 512, 167047	2.8	1
94	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	5.6	5
93	Structural and magnetic properties of Co-Pt clusters: A spin-polarized density functional study. *Journal of Magnetism and Magnetic Materials*, **2020**, 503, 166651	2.8	3
92	Solid□iquid Coexistence in Trimetallic Heterostructured Nanoparticle Catalysts: Insights from Molecular Dynamics Simulations. *ACS Applied Nano Materials*, **2020**, 3, 12369-12378	5.6	3
91	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	13	18
90	Effect of Chemical Ordering on Thermal Stability of Pt□o Nanoparticles. *Journal of Physical Chemistry C*, **2019**, 123, 12007-12014	3.8	9
89	GPU-based DPSO algorithm for structural optimization of Pt-Co bimetallic nanoparticles. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2019**, 383, 3123-3133	2.3	2
88	Thermally activated phase transitions in Fe-Ni core-shell nanoparticles. *Frontiers of Physics*, **2019**, 14, 1	3.7	

87	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	5.7	6
86	Shape Stability of Metallic Nanoplates: A Molecular Dynamics Study. *Nanoscale Research Letters*, **2019**, 14, 357	5	2
85	Spark-based improved Basin-Hopping Monte Carlo algorithm for structural optimization of alloy clusters. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2019**, 383, 464-470	2.3	4
84	Cluster-based niching differential evolution algorithm for optimizing the stable structures of metallic clusters. *Computational Materials Science*, **2018**, 149, 416-423	3.2	9
83	An improved genetic algorithm for structural optimization of Au$_n$Ag bimetallic nanoparticles. *Applied Soft Computing Journal*, **2018**, 73, 39-49	7.5	9
82	Direct observations of shape fluctuation in long-time atomistic simulations of metallic nanoclusters. *Physical Review Materials*, **2018**, 2,	3.2	6
81	Stable structure optimization of Pt-X-Cu (X = Au, Ag, Pd and Rh) trimetallic nanoparticles. *Journal of Alloys and Compounds*, **2017**, 716, 240-250	5.7	14
80	Thermal Stability of Platinum-Cobalt Bimetallic Nanoparticles: Chemically Disordered Alloys, Ordered Intermetallics, and Core-Shell Structures. *ACS Applied Materials & Interfaces*, **2017**, 9, 12486-12493	9.5	17
79	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	3.9	7
78	Thermal Stability of Co-Pt and Co-Au Core-Shell Structured Nanoparticles: Insights from Molecular Dynamics Simulations. *Journal of Physical Chemistry Letters*, **2017**, 8, 4273-4278	6.4	15
77	Robust indirect band gap and anisotropy of optical absorption in B-doped phosphorene. *Physical Chemistry Chemical Physics*, **2017**, 19, 31796-31803	3.6	14
76	Atomic structure and thermal stability of Pt-Fe bimetallic nanoparticles: from alloy to core/shell architectures. *Physical Chemistry Chemical Physics*, **2016**, 18, 17010-7	3.6	15
75	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	3	8
74	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	2.3	4
73	Structural optimization of Fe nanoclusters based on multi-populations differential evolution algorithm. *Journal of Nanoparticle Research*, **2016**, 18, 1	2.3	3
72	Atomic-scale insights into structural and thermodynamic stability of Pd-Ni bimetallic nanoparticles. *Physical Chemistry Chemical Physics*, **2016**, 18, 9847-54	3.6	12
71	Structural optimization of Pt$_n$Pd$_m$Rh trimetallic nanoparticles using improved genetic algorithm. *Journal of Alloys and Compounds*, **2016**, 663, 466-473	5.7	27
70	Structural and electronic properties of ZnO/GaN heterostructured nanowires from first-principles study. *Physical Chemistry Chemical Physics*, **2016**, 18, 3097-102	3.6	18

69	Structural optimization and segregation behavior of quaternary alloy nanoparticles based on simulated annealing algorithm. *Chinese Physics B*, **2016**, 25, 053601	1.2	1
68	Structure and stability of Fe-Pt bimetallic nanoparticles: Initial structure, composition and shape effects. *Journal of Alloys and Compounds*, **2016**, 685, 1008-1015	5.7	10
67	Could Borophene Be Used as a Promising Anode Material for High-Performance Lithium Ion Battery?. *ACS Applied Materials & Interfaces*, **2016**, 8, 22175-81	9.5	103
66	A multi-populations multi-strategies differential evolution algorithm for structural optimization of metal nanoclusters. *Computer Physics Communications*, **2016**, 208, 64-72	4.2	8
65	Structural optimization of PtPdAu trimetallic nanoparticles by discrete particle swarm algorithms. *Journal of Materials Science*, **2015**, 50, 3308-3319	4.3	23
64	Ultrawide photoresponse in ZnO/ZnSe coaxial nanowires with a threshold of 0.8eV. *International Journal of Hydrogen Energy*, **2015**, 40, 10788-10794	6.7	3
63	Structural optimization of PtPd alloy nanoparticles using an improved discrete particle swarm optimization algorithm. *Computer Physics Communications*, **2015**, 186, 11-18	4.2	13
62	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	3.8	2
61	Morphology and structural stability of PtPd bimetallic nanoparticles. *Chinese Physics B*, **2015**, 24, 033601	1.2	9
60	Structural studies of AuPd bimetallic nanoparticles by a genetic algorithm method. *Physica E: Low-Dimensional Systems and Nanostructures*, **2015**, 70, 11-20	3	8
59	Thermal and shape stability of high-index-faceted rhodium nanoparticles: a molecular dynamics investigation. *Physical Chemistry Chemical Physics*, **2015**, 17, 5751-7	3.6	10
58	Novel electronic structures of superlattice composed of graphene and silicene. *Materials Research Bulletin*, **2014**, 50, 268-272	5.1	10
57	Tetrahexahedral PtPd alloy nanocatalysts with high-index facets: an atomistic perspective on thermodynamic and shape stabilities. *Journal of Materials Chemistry A*, **2014**, 2, 1375-1382	13	14
56	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	13	21
55	Electrochemical synthesis of tetrahexahedral rhodium nanocrystals with extraordinarily high surface energy and high electrocatalytic activity. *Angewandte Chemie - International Edition*, **2014**, 53, 5097-101	16.4	106
54	Tunable thermodynamic stability of Au-CuPt core-shell trimetallic nanoparticles by controlling the alloy composition: insights from atomistic simulations. *Physical Chemistry Chemical Physics*, **2014**, 16, 22754-61	3.6	27
53	Single-crystalline and multiple-twinned gold nanoparticles: an atomistic perspective on structural and thermal stabilities. *RSC Advances*, **2014**, 4, 7528	3.7	21
52	Particle swarm optimization of the stable structure of tetrahexahedral Pt-based bimetallic nanoparticles. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2014**, 378, 2965-2972	2.3	5

51	Electrochemical Synthesis of Tetrahexahedral Rhodium Nanocrystals with Extraordinarily High Surface Energy and High Electrocatalytic Activity. *Angewandte Chemie*, **2014**, 126, 5197-5201	3.6	8
50	Diverse melting modes and structural collapse of hollow bimetallic core-shell nanoparticles: a perspective from molecular dynamics simulations. *Scientific Reports*, **2014**, 4, 7051	4.9	26
49	Structures and electronic properties of oxidized graphene from first-principles study. *Europhysics Letters*, **2014**, 105, 37005	1.6	7
48	Insights into electrochemical performance of Li2FeSiO4 from first-principles calculations. *Electrochimica Acta*, **2013**, 111, 172-178	6.7	26
47	Thermodynamic, structural and elastic properties of Co3X (X = Ti, Ta, W, V, Al) compounds from first-principles calculations. *Intermetallics*, **2013**, 32, 303-311	3.5	41
46	Structural and Electronic Properties of Superlattice Composed of Graphene and Monolayer MoS2. *Journal of Physical Chemistry C*, **2013**, 117, 15347-15353	3.8	88
45	Thermal Stability and Shape Evolution of Tetrahexahedral Au–Pd Core–Shell Nanoparticles with High-Index Facets. *Journal of Physical Chemistry C*, **2013**, 117, 6896-6903	3.8	25
44	Insight into the Melting Behavior of Au–Pt Core–Shell Nanoparticles from Atomistic Simulations. *Journal of Physical Chemistry C*, **2013**, 117, 4278-4286	3.8	53
43	First-Principles Investigations on the Na2MnPO4F as a Cathode Material for Na-Ion Batteries. *Journal of the Electrochemical Society*, **2013**, 160, A927-A932	3.9	26
42	Lower-Energy Structure Optimization of (C60)N Clusters Using an Improved Genetic Algorithm. *IEICE Transactions on Information and Systems*, **2013**, E96.D, 2726-2732	0.6	
41	First-Principles Investigation on the Lithium Ion Insertion/Extraction in Trirutile LixFeF3. *Electrochemistry*, **2013**, 81, 12-15	1.2	8
40	Pt–Pd Bimetallic Catalysts: Structural and Thermal Stabilities of Core–Shell and Alloyed Nanoparticles. *Journal of Physical Chemistry C*, **2012**, 116, 8664-8671	3.8	96
39	Enhanced thermal stability of Au@Pt nanoparticles by tuning shell thickness: Insights from atomistic simulations. *Journal of Materials Chemistry*, **2012**, 22, 7380		32
38	Two-Stage Melting in Core–Shell Nanoparticles: An Atomic-Scale Perspective. *Journal of Physical Chemistry C*, **2012**, 116, 11837-11841	3.8	42
37	First-principles studies on the structural and electronic properties of Li-ion battery cathode material CuF2. *Solid State Communications*, **2012**, 152, 1703-1706	1.6	13
36	Mechanical properties of platinum nanowires: An atomistic investigation on single-crystalline and twinned structures. *Computational Materials Science*, **2012**, 55, 205-210	3.2	23
35	Shape-Controlled Synthesis of Metal Nanoparticles of High Surface Energy and Their Applications in Electrocatalysis **2012**, 117-165		2
34	Structure and stability of platinum nanocrystals: from low-index to high-index facets. *Journal of Materials Chemistry*, **2011**, 21, 11578		57

33	Thermal stability of platinum nanowires: a comparison study between single-crystalline and twinned structures. *Journal of Materials Chemistry*, **2011**, 21, 18998		16
32	Magnetism of Mg atomic chains on the NaCl(100) surface. *Solid State Communications*, **2011**, 151, 1912-1915	1.6	1
31	Strain-tunable band gap of hydrogenated bilayer graphene. *New Journal of Physics*, **2011**, 13, 063047	2.9	15
30	Molecular dynamics investigation of structural evolution of fcc Fe nanoparticles under heating process. *Chemical Physics Letters*, **2011**, 502, 207-210	2.5	20
29	Electronic and magnetic properties of silicon adsorption on graphene. *Solid State Communications*, **2011**, 151, 1128-1130	1.6	15
28	Size-dependent elastic properties of single-walled ZnO nanotubes: A first-principles study. *Journal of Applied Physics*, **2011**, 109, 084325	2.5	9
27	Surface-passivation-induced metallic and magnetic properties of ZnO graphitic sheet. *Applied Physics Letters*, **2010**, 96, 223113	3.4	16
26	Structure and Stability of Fe Nanocrystals: An Atomistic Study. *Journal of Physical Chemistry C*, **2010**, 114, 18841-18846	3.8	24
25	Structural Design and Two-Dimensional Conductivity of Sheet-Tube Frameworks. *Journal of Physical Chemistry C*, **2010**, 114, 19673-19677	3.8	11
24	Comparative study of Cu13 and Co13 clusters deposition and diffusion on the Cu(001) surface. *Computational Materials Science*, **2010**, 48, 250-257	3.2	11
23	Orientation-dependent mechanical properties of Au nanowires under uniaxial loading. *Computational Materials Science*, **2010**, 48, 513-519	3.2	23
22	First-principles study on the structural and electronic properties of ultrathin ZnO nanofilms. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2010**, 374, 1054-1058	2.3	24
21	Strain-induced structural and direct-to-indirect band gap transition in ZnO nanotubes. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2010**, 374, 2846-2849	2.3	32
20	Compressive mechanical behavior of Au nanowires. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2010**, 374, 2949-2952	2.3	21
19	Magnetism of a free-standing W monoatomic sheet. *Solid State Sciences*, **2009**, 11, 2142-2148	3.4	1
18	Molecular dynamics investigation of shape effects on thermal characteristics of platinum nanoparticles. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2009**, 373, 272-276	2.3	40
17	Energetic and structural evolution of gold nanowire under heating process: A molecular dynamics study. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2009**, 373, 3454-3458	2.3	12
16	A molecular dynamics study of shape transformation and melting of tetrahexahedral platinum nanoparticle. *Chemical Physics Letters*, **2009**, 471, 295-299	2.5	36

15	Orientation-Dependent Structural Transition and Melting of Au Nanowires. *Journal of Physical Chemistry C*, **2009**, 113, 20611-20617	3.8	62
14	Direct to indirect band gap transition in ultrathin ZnO nanowires under uniaxial compression. *Applied Physics Letters*, **2009**, 94, 113114	3.4	48
13	Molecular dynamics study of the mechanical behavior of nickel nanowire: Strain rate effects. *Computational Materials Science*, **2008**, 41, 553-560	3.2	99
12	The elastic behavior in Ni monocrystal: Nonlinear effects. *Solid State Communications*, **2008**, 146, 253-257	1.6	9
11	Size-dependent effects on equilibrium stress and strain in nickel nanowires. *Physical Review B*, **2007**, 76,	3.3	23
10	Tolman Effect on Fluid Dynamics in Carbon Nanotubes. *Fullerenes Nanotubes and Carbon Nanostructures*, **2007**, 15, 417-426	1.8	1
9	TiNi Monatomic Chains Stabilized by Alloying: a First-Principles Study. *Chinese Physics Letters*, **2006**, 23, 182-185	1.8	5
8	The uniaxial tensile deformation of Ni nanowire: atomic-scale computer simulations. *Physica E: Low-Dimensional Systems and Nanostructures*, **2005**, 27, 113-120	3	38
7	Structural stabilities and electronic structures of Ti atomic chains. *Physica E: Low-Dimensional Systems and Nanostructures*, **2005**, 30, 138-142	3	14
6	A theoretical study of tunnelling conductance in ferromagnet/ PrOs4Sb12 junctions. *European Physical Journal B*, **2005**, 44, 137-143	1.2	
5	Surface-Induced Melting of Metal Nanoclusters. *Chinese Physics Letters*, **2004**, 21, 2171-2174	1.8	5
4	Size effects on the melting of nickel nanowires: a molecular dynamics study. *Physica E: Low-Dimensional Systems and Nanostructures*, **2004**, 25, 47-54	3	75
3	Molecular Dynamics Simulation of Microstructure of Nanocrystalline Copper. *Chinese Physics Letters*, **2001**, 18, 411-413	1.8	5
2	The influence of grain size and temperature on the mechanical deformation of nanocrystalline materials: molecular dynamics simulation. *Chinese Physics B*, **2001**, 10, 407-412		6
1	Molecular Dynamics Investigation on Thermal Stability and Shape Evolution of Pd-Au Heterostructured Nanorods: Implications for Catalysis. *ACS Applied Nano Materials*,	5.6	1