Liang-Feng Huang

List of Publications by Citations

65 papers	1,382 citations	21 h-index	35 g-index
67 ext. papers	1,650 ext. citations	5 avg, IF	5.02 L-index

#	Paper	IF	Citations
65	Correlation between structure, phonon spectra, thermal expansion, and thermomechanics of single-layer MoS2. *Physical Review B*, **2014**, 90,	3.3	102
64	Origin of shear induced β to ω transition in Ti Nb-based alloys. *Acta Materialia*, **2015**, 92, 55-63	8.4	98
63	Improved Electrochemical Phase Diagrams from Theory and Experiment: The Ni Water System and Its Complex Compounds. *Journal of Physical Chemistry C*, **2017**, 121, 9782-9789	3.8	92
62	Phonon properties, thermal expansion, and thermomechanics of silicene and germanene. *Physical Review B*, **2015**, 91,	3.3	77
61	Hydrogen storage in Li-doped charged single-walled carbon nanotubes. *International Journal of Hydrogen Energy*, **2010**, 35, 3546-3549	6.7	69
60	From electronic structure to phase diagrams: A bottom-up approach to understand the stability of titanium ransition metal alloys. *Acta Materialia*, **2016**, 113, 311-319	8.4	51
59	Modulation of the thermodynamic, kinetic, and magnetic properties of the hydrogen monomer on graphene by charge doping. *Journal of Chemical Physics*, **2011**, 135, 064705	3.9	49
58	Roles of Mass, Structure, and Bond Strength in the Phonon Properties and Lattice Anharmonicity of Single-Layer Mo and W Dichalcogenides. *Journal of Physical Chemistry C*, **2015**, 119, 18779-18789	3.8	46
57	Understanding the Protonation of Polyaniline and Polyaniline raphene Interaction. *Journal of Physical Chemistry C*, **2012**, 116, 13120-13126	3.8	44
56	An efficient ab-initio quasiharmonic approach for the thermodynamics of solids. *Computational Materials Science*, **2016**, 120, 84-93	3.2	43
55	Lattice dynamics and disorder-induced contraction in functionalized graphene. *Journal of Applied Physics*, **2013**, 113, 083524	2.5	40
54	Ab Initio Simulations of the Kinetic Properties of the Hydrogen Monomer on Graphene *Journal of Physical Chemistry C*, **2010**, 114, 22636-22643	3.8	38
53	Stabilizing the ground state in zigzag-edged graphene nanoribbons by dihydrogenation. *Physical Review B*, **2012**, 86,	3.3	38
52	Understanding the Band Gap, Magnetism, and Kinetics of Graphene Nanostripes in Graphane. *Journal of Physical Chemistry C*, **2011**, 115, 21088-21097	3.8	37
51	A Cluster Dynamics Model For Accumulation Of Helium In Tungsten Under Helium Ions And Neutron Irradiation. *Communications in Computational Physics*, **2012**, 11, 1547-1568	2.4	35
50	Electrochemical phase diagrams for Ti oxides from density functional calculations. *Physical Review B*, **2015**, 92,	3.3	31
49	Modeling Corrosion with First-Principles Electrochemical Phase Diagrams. *Annual Review of Materials Research*, **2019**, 49, 53-77	12.8	30

48	Localized Symmetry Breaking for Tuning Thermal Expansion in ScF Nanoscale Frameworks. *Journal of the American Chemical Society*, **2018**, 140, 4477-4480	16.4	26
47	Cluster dynamics modeling of accumulation and diffusion of helium in neutron irradiated tungsten. *Journal of Nuclear Materials*, **2012**, 431, 26-32	3.3	26
46	Importance of coordination number and bond length in titanium revealed by electronic structure investigations. *Physica Status Solidi (B): Basic Research*, **2015**, 252, 1907-1924	1.3	22
45	Role of 2D and 3D defects on the reduction of LaNiO nanoparticles for catalysis. *Scientific Reports*, **2017**, 7, 10080	4.9	21
44	Orbital symmetry induced conductance switching in a graphene nanoribbon heterojunction with different edge hydrogenations. *Applied Physics Letters*, **2012**, 101, 053101	3.4	21
43	Band gap engineering in armchair-edged graphene nanoribbons by edge dihydrogenation. *Computational Materials Science*, **2012**, 62, 93-98	3.2	21
42	Understanding and tuning the quantum-confinement effect and edge magnetism in zigzag graphene nanoribbon. *Journal of Physics Condensed Matter*, **2013**, 25, 055304	1.8	20
41	Tuning the adatom-surface and interadatom interactions in hydrogenated graphene by charge doping. *Physical Review B*, **2012**, 86,	3.3	20
40	Tunable Negative Thermal Expansion in Layered Perovskites from Quasi-Two-Dimensional Vibrations. *Physical Review Letters*, **2016**, 117, 115901	7.4	20
39	Isotope effects on the vibrational, Invar, and Elinvar properties of pristine and hydrogenated graphene. *Solid State Communications*, **2014**, 190, 5-9	1.6	19
38	Reliable electrochemical phase diagrams of magnetic transition metals and related compounds from high-throughput ab initio calculations. *Npj Materials Degradation*, **2019**, 3,	5.7	18
37	Friction and Wear Behavior of CrN Coating on 316L Stainless Steel in Liquid Sodium at Elevated Temperature. *Tribology International*, **2020**, 143, 106079	4.9	17
36	Dynamical behaviors of self-interstitial atoms in tungsten. *Journal of Nuclear Materials*, **2013**, 437, 438-444	3.3	15
35	Contrasting Oxygen Reduction Reactions on Zero- and One-Dimensional Defects of MoS for Versatile Applications. *ACS Applied Materials & Interfaces*, **2019**, 11, 46327-46336	9.5	14
34	Robust and Pristine Topological Dirac Semimetal Phase in Pressured Two-Dimensional Black Phosphorus. *Journal of Physical Chemistry C*, **2017**, 121, 20931-20936	3.8	12
33	Patterning graphene nanostripes in substrate-supported functionalized graphene: A promising route to integrated, robust, and superior transistors. *Frontiers of Physics*, **2012**, 7, 324-327	3.7	12
32	Superhydrophilic Fe Doped TiO Films with Long-Lasting Antifogging Performance. *ACS Applied Materials & Interfaces*, **2021**, 13, 3377-3386	9.5	12
31	Electrochemical phase diagrams of Ni from ab initio simulations: role of exchange interactions on accuracy. *Journal of Physics Condensed Matter*, **2017**, 29, 475501	1.8	10

30	The thermodynamic and kinetic properties of hydrogen dimers on graphene. *Surface Science*, **2011**, 605, 1489-1496	1.8	10
29	Structure Dependent Phase Stability and Thermal Expansion of Ruddlesden–Popper Strontium Titanates. *Chemistry of Materials*, **2018**, 30, 7100-7110	9.6	10
28	Multifunctional two-dimensional semiconductors SnP: universal mechanism of layer-dependent electronic phase transition. *Journal of Physics Condensed Matter*, **2018**, 30, 475702	1.8	9
27	Hydrogen-Coverage-Dependent Stark Effect in Bilayer Graphene and Graphene/BN Nanofilms. *Journal of Physical Chemistry C*, **2014**, 118, 10472-10480	3.8	8
26	Catalytic Enhancement of CO Oxidation on LaFeO Regulated by Ruddlesden-Popper Stacking Faults. *ACS Applied Materials & Interfaces*, **2019**, 11, 33850-33858	9.5	7
25	The Accumulation of He on a W Surface During keV-He Irradiation: Cluster Dynamics Modeling. *Plasma Science and Technology*, **2012**, 14, 624-628	1.5	7
24	Chemical optimization towards superior electrocatalysis of Janus 1T-MoSX (X = O, Se, Te) for hydrogen evolution: Small composition tuning makes big difference. *Electrochimica Acta*, **2019**, 310, 153-161	6.7	6
23	Stable zigzag edges of transition-metal dichalcogenides with high catalytic activity for oxygen reduction. *Electrochimica Acta*, **2020**, 338, 135865	6.7	6
22	Theoretical simulation of thermal behavior in transient heat loads testing of plasma-facing materials. *Fusion Engineering and Design*, **2011**, 86, 2812-2820	1.7	6
21	Layer-by-layer stacked graphene nanocoatings by Marangoni self-assembly for corrosion protection of stainless steel. *Chinese Chemical Letters*, **2021**, 32, 501-505	8.1	6
20	Crystal Orientation-Dependent Oxidation of Epitaxial TiN Films with Tunable Plasmonics. *ACS Photonics*, **2021**, 8, 847-856	6.3	6
19	Thermodynamics and kinetics of an oxygen adatom on pristine and functionalized graphene: insight gained into their anticorrosion properties. *Physical Chemistry Chemical Physics*, **2019**, 21, 12121-12129	3.6	5
18	Nonlocal and Local Electrochemical Effects of Doping Impurities on the Reactivity of Graphene. *Journal of Physical Chemistry C*, **2015**, 119, 10513-10519	3.8	5
17	Understanding the stability and dynamical process of hydrogen trimers on graphene. *Journal of Applied Physics*, **2013**, 113, 173707	2.5	5
16	Physical spread and technical upshift in the band gaps of visible-light photocatalytic bismuth oxyhalide solid solutions. *Computational Materials Science*, **2020**, 184, 109870	3.2	5
15	Highly in-plane anisotropic 2D semiconductors AuSe with multiple superior properties: a first-principles investigation. *Journal of Physics Condensed Matter*, **2019**, 31, 395501	1.8	4
14	The diffusion of hydrogen monomers on hole-doped graphitic lattices: over-barrier transition and quantum tunneling. *Journal of Physics Condensed Matter*, **2011**, 23, 435007	1.8	4
13	Understanding Electrochemical Stabilities of Ni-Based Nanofilms from a Comparative Theory–Experiment Approach. *Journal of Physical Chemistry C*, **2019**, 123, 28925-28940	3.8	4

12	Unraveling the strong coupling between graphene/nickel interface and atmospheric adsorbates for versatile realistic applications. *Carbon Trends*, **2021**, 2, 100013	0	4
11	Stable MoSi2 nanofilms with controllable and high metallicity. *Physical Review Materials*, **2017**, 1,	3.2	3
10	Correlated morphological and chemical mechanisms for the superior corrosion resistance of alumina-deposited 2D nanofilms on copper. *Materialia*, **2020**, 11, 100697	3.2	3
9	The mechanisms of impurity□mpurity and impurity□atrix interactions in B/N-doped graphene. *Chemical Physics Letters*, **2014**, 605-606, 56-61	2.5	2
8	Adsorption configurations and scanning voltage determined STM images of small hydrogen clusters on bilayer graphene. *Journal of Chemical Physics*, **2013**, 139, 194708	3.9	2
7	First-Principles-Based Prediction of Electrochemical Oxidation and Corrosion of Copper under Multiple Environmental Factors. *Journal of Physical Chemistry C*, **2021**, 125, 14027-14038	3.8	2
6	Construction of hierarchical nanocarrier via a □MOFs plus graphene□strategy for sustained release and rust-induced self-healing. *Chemical Engineering Journal*, **2021**, 426, 131879	14.7	2
5	Negative thermal expansion in the Ruddlesden-Popper calcium titanates. *Physical Review Materials*, **2021**, 5,	3.2	1
4	Corrosion Resistance of Ultrathin Two-Dimensional Coatings: First-Principles Calculations towards In-Depth Mechanism Understanding and Precise Material Design. *Metals*, **2021**, 11, 2011	2.3	1
3	Eliminating the Galvanic Corrosion Effect of Graphene Coating by an Accurate and Rapid Self-Assembling Defect Healing Approach. *Advanced Functional Materials*, **2022**, 32, 2110264	15.6	1
2	A Green Strategy for Nitrogen-Doped Polymer Nanodots with High Oxygen and Chloride Corrosion Resistance in Extremely Acidic Condition. *Chemical Engineering Journal*, **2022**, 437, 135242	14.7	0
1	Electrochemical catalysis and corrosion of defective MoS2: Microscopic behaviors and density-functional-theory calculations. *Current Opinion in Electrochemistry*, **2022**, 101008	7.2	