Wang-Yu Hu

List of Publications by Year in Descending Order

388 papers	6,195 citations	39 h-index	58 g-index
402 ext. papers	7,281 ext. citations	3.6 avg, IF	6.08 L-index

#	Paper	IF	Citations
388	Solidification of Undercooled Liquid under Supergravity Field by Phase-Field Crystal Approach. *Metals*, **2022**, 12, 232	2.3	0
387	Molecular dynamic simulations of plasticity and phase transition in Mg polycrystalline under shock compression. *Applied Physics Express*, **2022**, 15, 015503	2.4	2
386	Critical structural invariant during high-pressure solidification of copper. *MRS Communications*, **2022**, 12, 45	2.7	0
385	Effect of Vacancies on Dynamic Response and Spallation in Single-Crystal Magnesium by Molecular Dynamic Simulation. *Metals*, **2022**, 12, 215	2.3	
384	Synergistic Effects of Crystal Phase and Strain for N Dissociation on Ru(0001) Surfaces with Multilayered Hexagonal Close-Packed Structures.. *ACS Omega*, **2022**, 7, 4492-4500	3.9	1
383	Two-dimensional chromium phosphorus monolayer based gas sensors to detect NOx: A first-principles study. *Results in Physics*, **2022**, 32, 105100	3.7	0
382	Effect of nanopores on plasticity and their collapse mechanism in magnesium single crystal under shock loading. *Journal of Applied Physics*, **2022**, 131, 055903	2.5	1
381	Molecular dynamic simulations of displacement cascades in tungsten and tungsten□henium alloys: Effects of grain boundary and/or □phase. *Journal of Nuclear Materials*, **2022**, 561, 153543	3.3	1
380	Influence of orientation on crack propagation of aluminum by molecular dynamics. *European Physical Journal B*, **2022**, 95, 1	1.2	
379	Crystallographic-orientation-dependence plasticity of niobium under shock compressions. *International Journal of Plasticity*, **2022**, 150, 103195	7.6	0
378	The mechanism of plasticity and phase transition in iron single crystals under cylindrically divergent shock loading. *International Journal of Mechanical Sciences*, **2022**, 217, 107032	5.5	1
377	A host□guest self-assembly strategy to enhance □electron densities in ultrathin porous carbon nitride nanocages toward highly efficient hydrogen evolution. *Chemical Engineering Journal*, **2022**, 430, 132880	14.7	7
376	Atomistic simulation on the generation of defects in Cu/SiC composites during cooling. *Journal of Materials Science and Technology*, **2022**, 123, 1-12	9.1	0
375	Pt-based intermetallic compounds with tunable activity and selectivity toward hydrogen production from formic acid. *Applied Surface Science*, **2022**, 153530	6.7	1
374	Effects of Point Defects on the Stable Occupation, Diffusion and Nucleation of Xe and Kr in UO2. *Metals*, **2022**, 12, 789	2.3	1
373	Orientation dependence of shock-induced change of habit plane for the 1/2<111> dislocation loop and plasticity in tungsten. *International Journal of Plasticity*, **2022**, 155, 103329	7.6	0
372	Effect of crystallographic orientations on shock-induced plasticity for CoCrFeMnNi high-entropy alloy. *International Journal of Mechanical Sciences*, **2022**, 107373	5.5	1

371	The Role of Grain Boundaries in the Corrosion Process of Fe Surface: Insights from ReaxFF Molecular Dynamic Simulations. *Metals*, **2022**, 12, 876	2.3	1
370	Shock-induced plasticity and phase transformation in single crystal magnesium: An interatomic potential and non-equilibrium molecular dynamics simulations.. *Journal of Physics Condensed Matter*, **2021**,	1.8	3
369	Dipole Engineering of Two-Dimensional van der Waals Heterostructures for Enhanced Power-Conversion Efficiency: The Case of Janus Ga2SeTe/InS. *Physical Review Applied*, **2021**, 16,	4.3	5
368	Study on the effect of non-centrosymmetric orientation in shocked and ramp compressed □ron. *Materials Today Communications*, **2021**, 29, 102893	2.5	
367	Highly effective Ru-based Heusler alloy catalysts for N2 activation: A theoretical study. *Applied Surface Science*, **2021**, 151658	6.7	1
366	The interactions between nitrogen oxides and □uranium surface. *Nuclear Materials and Energy*, **2021**, 26, 100945	2.1	
365	High-Throughput One-Photon Excitation Pathway in 0D/3D Heterojunctions for Visible-Light Driven Hydrogen Evolution. *Advanced Functional Materials*, **2021**, 31, 2100816	15.6	40
364	Effects of Se substitution on the Schottky barrier of a MoS x Se(2□)/graphene heterostructure. *Journal Physics D: Applied Physics*, **2021**, 54, 265302	3	2
363	One-Photon Excitation Pathway: High-Throughput One-Photon Excitation Pathway in 0D/3D Heterojunctions for Visible-Light Driven Hydrogen Evolution (Adv. Funct. Mater. 18/2021). *Advanced Functional Materials*, **2021**, 31, 2170125	15.6	
362	Energetics and diffusional properties of helium in W-Ta systems studied by a new ternary potential. *Journal of Nuclear Materials*, **2021**, 549, 152913	3.3	1
361	First-principles study on the dissolution and diffusion behavior of hydrogen in carbide precipitates. *International Journal of Hydrogen Energy*, **2021**, 46, 22030-22039	6.7	2
360	Atomistic insights into interactions between oxygen and □r (101-1) surface. *Nuclear Materials and Energy*, **2021**, 27, 100974	2.1	
359	Molecular dynamics simulation of shock wave propagation and spall failure in single crystal copper under cylindrical impact. *Applied Physics Express*, **2021**, 14, 075504	2.4	2
358	Predicted Polymeric and Layered Covalent Networks in Transition Metal Pentazolate M(cyclo-N5)x Phases at Ambient and High Pressure: Up to 20 Nitrogen Atoms per Metal. *Chemistry of Materials*, **2021**, 33, 5298-5307	9.6	0
357	2D Amorphous CoO Incorporated g-C3N4 Nanotubes for Improved Photocatalytic Performance. *Physica Status Solidi - Rapid Research Letters*, **2021**, 15, 2100254	2.5	2
356	Unsaturated coordination polymer frameworks as multifunctional sulfur reservoir for fast and durable lithium-sulfur batteries. *Nano Energy*, **2021**, 79, 105393	17.1	22
355	A two-dimensional MoS2/SnS heterostructure for promising photocatalytic performance: First-principles investigations. *Physica E: Low-Dimensional Systems and Nanostructures*, **2021**, 126, 114453	3	3
354	Assessing Atomic-Phase Transitions and Ion Transport in Layered NaxNiO2 (x □0.67) Cathode Materials. *Journal of Physical Chemistry C*, **2021**, 125, 4930-4937	3.8	

353	Strain and interfacial engineering to accelerate hydrogen evolution reaction of two-dimensional phosphorus carbide*. *Chinese Physics B*, **2021**, 30, 027101	1.2	0
352	Effects of vacancies on plasticity and phase transformation in single-crystal iron under shock loading. *Journal of Applied Physics*, **2021**, 130, 015107	2.5	1
351	High-throughput computational design for 2D van der Waals functional heterostructures: Fragility of Andersonꞌs rule and beyond. *Applied Physics Letters*, **2021**, 119, 043102	3.4	10
350	Unraveling TM Migration Mechanisms in LiNiMnCoO by Modeling and Experimental Studies. *Nano Letters*, **2021**, 21, 6875-6881	11.5	6
349	Effects of electric field and strain on the Schottky barrier of the bilayer van der Waals heterostructures of graphene and pure/hydrogenated PC3 monolayer. *Physica E: Low-Dimensional Systems and Nanostructures*, **2021**, 133, 114785	3	0
348	Molecular dynamics simulation of the behavior of typical radiation defects under stress gradient field in tungsten. *Journal of Applied Physics*, **2021**, 130, 125103	2.5	0
347	Monolayer PtTe2: A promising candidate for NO2 sensor with ultrahigh sensitivity and selectivity. *Physica E: Low-Dimensional Systems and Nanostructures*, **2021**, 134, 114925	3	2
346	Effect of transition metal atoms on the stacking fault energy and ductility of TiC. *Ceramics International*, **2021**, 47, 29386-29391	5.1	1
345	Atomistic simulation of the surface configuration of the NiRe cluster. *Thin Solid Films*, **2021**, 737, 138938	2.2	
344	Molecular dynamics simulation of primary radiation damage in W-Ta alloys: Effect of tantalum. *Journal of Nuclear Materials*, **2021**, 556, 153162	3.3	3
343	FinnisSinclair-type potential for atomistic simulation of defects behaviour in V-Ti-Ta ternary system. *Journal of Nuclear Materials*, **2021**, 557, 153231	3.3	1
342	Generalized Synthetic Strategy for Amorphous Transition Metal Oxides-Based 2D Heterojunctions with Superb Photocatalytic Hydrogen and Oxygen Evolution. *Advanced Functional Materials*, **2021**, 31, 2009230	15.6	45
341	Chemistry of Defects in Crystalline Na2Se: Implications for the NaSe Battery. *Journal of Physical Chemistry C*, **2020**, 124, 27930-27936	3.8	3
340	Effect of symmetrical tilt grain boundary on the compatibility between copper and liquid lithium: Atomistic simulations. *Journal of Alloys and Compounds*, **2020**, 835, 155212	5.7	0
339	Ultra-thin tubular graphitic carbon Nitride-Carbon Dot lateral heterostructures: One-Step synthesis and highly efficient catalytic hydrogen generation. *Chemical Engineering Journal*, **2020**, 397, 125470	14.7	38
338	Molecular dynamics simulation of cylindrically converging shock response in single crystal Cu. *Computational Materials Science*, **2020**, 183, 109845	3.2	4
337	Molecular dynamics simulations of the diffusion characteristics on the Fe-W interfaces system. *Fusion Engineering and Design*, **2020**, 159, 111850	1.7	3
336	Dynamic self-diffusion behaviors of nickel adatoms on clusters with Wulff shape. *International Journal of Modern Physics B*, **2020**, 34, 2050015	1.1	1

335	Enhanced radiation tolerance of the Ni-Co-Cr-Fe high-entropy alloy as revealed from primary damage. *Acta Materialia*, **2020**, 196, 133-143	8.4	45
334	Structural damage and phase stability of Al0.3CoCrFeNi high entropy alloy under high temperature ion irradiation. *Acta Materialia*, **2020**, 188, 1-15	8.4	42
333	Carbide effects on tensile deformation behavior of [001] symmetric tilt grain boundaries in bcc Fe. *Modelling and Simulation in Materials Science and Engineering*, **2020**, 28, 035006	2	1
332	Hierarchical Self-assembly of Well-Defined Louver-Like P-Doped Carbon Nitride Nanowire Arrays with Highly Efficient Hydrogen Evolution. *Nano-Micro Letters*, **2020**, 12, 52	19.5	24
331	A comparative atomic simulation study of the configurations in M-Al (M = Mg, Ni, and Fe) nanoalloys: influence of alloying ability, surface energy, atomic radius, and atomic arrangement. *Journal of Nanoparticle Research*, **2020**, 22, 1	2.3	2
330	Molecular dynamics simulations of radiation damage generation and dislocation loop evolution in Ni and binary Ni-based alloys. *Computational Materials Science*, **2020**, 177, 109555	3.2	5
329	From monolayer to lateral heterostructure of functionalized phosphorus carbide: Evolution of electronic properties. *Physica E: Low-Dimensional Systems and Nanostructures*, **2020**, 118, 113962	3	4
328	Double-Layer Honeycomb AlP: A Promising Anode Material for Li-, Na-, and K-Ion Batteries. *Journal of Physical Chemistry C*, **2020**, 124, 2978-2986	3.8	5
327	A design rule for two-dimensional van der Waals heterostructures with unconventional band alignments. *Physical Chemistry Chemical Physics*, **2020**, 22, 3037-3047	3.6	12
326	Interatomic potentials of W–V and W–Mo binary systems for point defects studies. *Journal of Nuclear Materials*, **2020**, 531, 152020	3.3	5
325	Atomic simulation of mechanical properties of irradiated iron. *International Journal of Modern Physics C*, **2020**, 31, 2050027	1.1	1
324	Evaluation of tungsten interatomic potentials for radiation damage simulations. *Tungsten*, **2020**, 2, 3-14	4.6	3
323	Strain and Electric Field Controllable Schottky Barriers and Contact Types in Graphene-MoTe van der Waals Heterostructure. *Nanoscale Research Letters*, **2020**, 15, 180	5	10
322	Interaction between impurity elements (C, N and O) and hydrogen in hcp-Zr: a first-principles study. *Modelling and Simulation in Materials Science and Engineering*, **2020**, 28, 085007	2	
321	Comparative investigation of microjetting from tin surface subjected to laser and plane impact loadings via molecular dynamics simulations. *Mechanics of Materials*, **2020**, 148, 103479	3.3	1
320	Molecular dynamics simulation of the interactions between screw dislocation and stacking fault tetrahedron in $Fe_{70}Ni_{20}Cr$ and Ni. *Modelling and Simulation in Materials Science and Engineering*, **2020**, 28, 075002	2	2
319	In situ construction of hierarchical graphitic carbon nitride homojunction as robust bifunctional photoelectrocatalyst for overall water splitting. *Journal of Chemical Technology and Biotechnology*, **2020**, 95, 758-769	3.5	5
318	Interfacial charge modulation: carbon quantum dot implanted carbon nitride double-deck nanoframes for robust visible-light photocatalytic tetracycline degradation. *Nanoscale*, **2020**, 12, 3135-3145	7.7	24

317	Ultrahigh Sensitivity and Selectivity of Pentagonal SiC2 Monolayer Gas Sensors: The Synergistic Effect of Composition and Structural Topology. *Physica Status Solidi (B): Basic Research*, **2020**, 257, 1900445	1.3	3
316	Atomistic simulations of the interaction between transmutation-produced Re and grain boundaries in tungsten. *Computational Materials Science*, **2020**, 173, 109412	3.2	4
315	Algorithm for generating irreducible site-occupancy configurations. *Physical Review B*, **2020**, 102,	3.3	1
314	Interatomic potentials and defect properties of FeCrAl alloys. *Journal of Nuclear Materials*, **2020**, 541, 152421	3.3	6
313	The phase transition of rapidly super-cooled Tungsten under 100 GPa. *Chemical Physics Letters*, **2020**, 755, 137789	2.5	1
312	Molecular dynamics simulation of the diffusion of self-interstitial atoms and interstitial loops under temperature gradient field in tungsten. *Journal of Applied Physics*, **2020**, 128, 065103	2.5	4
311	Molecular dynamics simulations of shock loading of nearly fully dense granular Ni-Al composites. *Physical Chemistry Chemical Physics*, **2019**, 21, 20252-20261	3.6	3
310	Assessment of van der Waals inclusive density functional theory methods for adsorption and selective dehydrogenation of formic acid on Pt(111) surface. *Physical Chemistry Chemical Physics*, **2019**, 21, 21049-21056	3.6	15
309	Influence of Irradiation on Mechanical Properties of Nickel. *Advances in Materials Science and Engineering*, **2019**, 2019, 1-6	1.5	
308	Precipitate/vanadium interface and its strengthening on the vanadium alloys: A first-principles study. *Journal of Nuclear Materials*, **2019**, 527, 151821	3.3	7
307	Molecular dynamics simulations of high-energy radiation damage in W and WRe alloys. *Journal of Nuclear Materials*, **2019**, 524, 9-20	3.3	12
306	Chlorine doped graphitic carbon nitride nanorings as an efficient photoresponsive catalyst for water oxidation and organic decomposition. *Journal of Materials Science and Technology*, **2019**, 35, 2288-2296	9.1	40
305	Tunable Schottky barrier in van der Waals heterostructures of graphene and hydrogenated phosphorus carbide monolayer: first-principles calculations. *Journal Physics D: Applied Physics*, **2019**, 52, 305104	3	10
304	The interactions between rhenium and interstitial-type defects in bulk tungsten: A combined study by molecular dynamics and molecular statics simulations. *Journal of Nuclear Materials*, **2019**, 522, 200-211	3.3	16
303	Doping-induced enhancement of crystallinity in polymeric carbon nitride nanosheets to improve their visible-light photocatalytic activity. *Nanoscale*, **2019**, 11, 6876-6885	7.7	93
302	Doping-Induced Hydrogen-Bond Engineering in Polymeric Carbon Nitride To Significantly Boost the Photocatalytic H Evolution Performance. *ACS Applied Materials & Interfaces*, **2019**, 11, 17341-17349	9.5	46
301	Understanding the release of helium atoms from nanochannel tungsten: a molecular dynamics simulation. *Nuclear Fusion*, **2019**, 59, 076020	3.3	7
300	Effect of MCl3 (M=La, U or Sc) component on the local structures and transport properties of LiCl-KCl-MCl3 eutectic: A molecular dynamics study. *Electrochimica Acta*, **2019**, 306, 366-376	6.7	8

299	Development of a NiMo interatomic potential for irradiation simulation. *Modelling and Simulation in Materials Science and Engineering*, **2019**, 27, 045009	2	4
298	Development of the interatomic potentials for W-Ta system. *Computational Materials Science*, **2019**, 163, 91-99	3.2	10
297	Protonated supramolecular complex-induced porous graphitic carbon nitride nanosheets as bifunctional catalyst for water oxidation and organic pollutant degradation. *Journal of Materials Science*, **2019**, 54, 7637-7650	4.3	9
296	Intrinsic strain-induced segregation in multiply twinned Cu-Pt icosahedra. *Physical Chemistry Chemical Physics*, **2019**, 21, 4802-4809	3.6	6
295	Atomistic insights into the reaction mechanism of nanostructured LiI: Implications for rechargeable Li-I2 batteries. *Energy Storage Materials*, **2019**, 17, 211-219	19.4	7
294	Clustering and dislocation loop punching induced by different noble gas bubbles in tungsten: a molecular dynamics study. *Modelling and Simulation in Materials Science and Engineering*, **2019**, 27, 084002	2	0
293	Theoretical insights into nitrogen fixation on Ti2C and Ti2CO2 in a lithium–nitrogen battery. *Journal of Materials Chemistry A*, **2019**, 7, 19950-19960	13	10
292	Interactions of plasticity and phase transformation under shock in iron bicrystals. *Journal of Applied Physics*, **2019**, 126, 045901	2.5	4
291	Strategy to boost catalytic activity of polymeric carbon nitride: synergistic effect of controllable in situ surface engineering and morphology. *Nanoscale*, **2019**, 11, 16393-16405	7.7	33
290	Monolayer Phosphorene-Carbon Nanotube Heterostructures for Photocatalysis: Analysis by Density Functional Theory. *Nanoscale Research Letters*, **2019**, 14, 233	5	3
289	Steering charge kinetics boost the photocatalytic activity of graphitic carbon nitride: heteroatom-mediated spatial charge separation and transfer. *Journal Physics D: Applied Physics*, **2019**, 53, 015502	3	23
288	Effect of particle packing and density on shock response in ordered arrays of Ni + Al nanoparticles. *Physical Chemistry Chemical Physics*, **2019**, 21, 7272-7280	3.6	7
287	Shock-induced migration of asymmetry tilt grain boundary in iron bicrystal: A case study of Σ [110]. *Chinese Physics B*, **2019**, 28, 126201	1.2	1
286	Electrostatic Potential Anomaly in 2D Janus Transition Metal Dichalcogenides. *Annalen Der Physik*, **2019**, 531, 1900369	2.6	8
285	Penta-Graphene as a Potential Gas Sensor for NO Detection. *Nanoscale Research Letters*, **2019**, 14, 306	5	28
284	Two-Dimensional GaX/SnS2 (X = S, Se) van der Waals Heterostructures for Photovoltaic Application: Heteroatom Doping Strategy to Boost Power Conversion Efficiency. *Physica Status Solidi - Rapid Research Letters*, **2019**, 13, 1800565	2.5	27
283	Atomistic studies of shock-induced plasticity and phase transition in iron-based single crystal with edge dislocation. *International Journal of Plasticity*, **2019**, 114, 215-226	7.6	24
282	Revealing the Reaction Mechanism of Sodium Selenide Confined within a Single-Walled Carbon Nanotube: Implications for Na-Se Batteries. *ACS Applied Materials & Interfaces*, **2019**, 11, 4995-5002	9.5	19

281	Isotype heterojunction g-C3N4/g-C3N4 nanosheets as 2D support to highly dispersed 0D metal oxide nanoparticles: Generalized self-assembly and its high photocatalytic activity. *Journal Physics D: Applied Physics*, **2019**, 52, 025501	3	36
280	The effect of Mo addition on structure and glass forming ability of Ni-Zr alloys. *Journal of Alloys and Compounds*, **2019**, 775, 1184-1198	5.7	17
279	Molecular dynamics simulation of alloying during sintering of Li and Pb metallic nanoparticles. *Computational Materials Science*, **2019**, 156, 47-55	3.2	17
278	Insights Into Interfacial Interaction and Its Influence on the Electronic and Optical Properties of Two-Dimensional WS2/TX2CO2 (TX = Ti, Zr) van der Waals Heterostructures. *Physica Status Solidi (B): Basic Research*, **2019**, 256, 1800377	1.3	1
277	Effect of temperature on the corrosion behaviors of 304 stainless steel in static liquid lithium. *Fusion Engineering and Design*, **2018**, 128, 75-81	1.7	13
276	Self-assembled hierarchical carbon/g-C3N4 composite with high photocatalytic activity. *Journal Physics D: Applied Physics*, **2018**, 51, 135501	3	9
275	Evolution of helium bubbles below different tungsten surfaces under neutron irradiation and non-irradiation conditions. *Computational Materials Science*, **2018**, 148, 242-248	3.2	11
274	Interfacial Interaction between Boron Cluster and Metal Oxide Surface and Its Effects: A Case Study of B20/Ag3PO4 van der Waals Heterostructure. *Journal of Physical Chemistry C*, **2018**, 122, 6151-6158	3.8	7
273	Wetting characteristics of lithium droplet on iron surfaces in atomic scale: A molecular dynamics simulation. *Computational Materials Science*, **2018**, 149, 435-441	3.2	2
272	Revealing reaction mechanisms of nanoconfined LiS: implications for lithium-sulfur batteries. *Physical Chemistry Chemical Physics*, **2018**, 20, 11713-11721	3.6	18
271	New interatomic potentials of W, Re and W-Re alloy for radiation defects. *Journal of Nuclear Materials*, **2018**, 502, 141-153	3.3	35
270	Effect of grain boundaries on shock-induced phase transformation in iron bicrystals. *Journal of Applied Physics*, **2018**, 123, 045105	2.5	19
269	A first-principles investigation of the ScO2 monolayer as the cathode material for alkali metal-ion batteries. *Journal of Materials Chemistry A*, **2018**, 6, 3171-3180	13	15
268	Oxygen adsorption and diffusion on □U(0 0 1) surface: Effect of titanium. *Computational Materials Science*, **2018**, 144, 85-91	3.2	6
267	An ab initio study for probing iodization reactions on metallic anode surfaces of Li□2 batteries. *Journal of Materials Chemistry A*, **2018**, 6, 7807-7814	13	6
266	Molecular dynamics simulations of the characteristics of Mo/Ti interfaces. *Computational Materials Science*, **2018**, 141, 293-301	3.2	16
265	In-situ construction of 2D direct Z-scheme g-C3N4/g-C3N4 homojunction with high photocatalytic activity. *Journal of Materials Science*, **2018**, 53, 15882-15894	4.3	33
264	Substrate-induced magnetism and topological phase transition in silicene. *Nanoscale*, **2018**, 10, 14667-14677	7	9

263	Simultaneous dispersive and covalent monolayer MoS2/TiO2 cluster heterostructures: Insights into their enhanced photocatalytic activity. *Superlattices and Microstructures*, **2018**, 121, 64-74	2.8	
262	Compatibility of Molybdenum, Tungsten, and 304 Stainless Steel in Static Liquid Lithium Under High Vacuum. *Plasma Physics Reports*, **2018**, 44, 671-677	1.2	3
261	Theoretical prediction of LiScO nanosheets as a cathode material for Li-O batteries. *Physical Chemistry Chemical Physics*, **2018**, 20, 22351-22358	3.6	6
260	Effect of neon on the hydrogen behaviors in tungsten: A first-principles study. *Journal of Nuclear Materials*, **2018**, 510, 492-498	3.3	2
259	Surface segregation and alloying of immiscible Li-Cu and miscible Li-Pb nanoalloys investigated by basin-hopping Monte Carlo method. *Computational Materials Science*, **2018**, 154, 371-379	3.2	4
258	Modified analytic embedded atom method potential for chromium. *Modelling and Simulation in Materials Science and Engineering*, **2018**, 26, 065001	2	2
257	Local identification of chemical ordering: Extension, implementation, and application of the common neighbor analysis for binary systems. *Computational Materials Science*, **2018**, 143, 195-205	3.2	3
256	Interfacial Interactions in Monolayer and Few-Layer SnS/CH NH PbI Perovskite van der Waals Heterostructures and Their Effects on Electronic and Optical Properties. *ChemPhysChem*, **2018**, 19, 291-299	3.3	12
255	Investigation of the interstitial oxygen behaviors in vanadium alloy: A first-principles study. *Current Applied Physics*, **2018**, 18, 183-190	2.6	11
254	Does the MgI2 Battery Suffer Severe Shuttle Effect?. *Journal of Physical Chemistry C*, **2018**, 122, 28518-28527	3.3	3
253	Theory-Driven Heterojunction Photocatalyst Design with Continuously Adjustable Band Gap Materials. *Journal of Physical Chemistry C*, **2018**, 122, 28065-28074	3.8	17
252	Atomic scale analysis of the corrosion characteristics of Cu-Li solid-liquid interfaces. *Journal of Alloys and Compounds*, **2018**, 763, 1-10	5.7	5
251	Facile in situ construction of mediator-free direct Z-scheme g-C3N4/CeO2 heterojunctions with highly efficient photocatalytic activity. *Journal Physics D: Applied Physics*, **2018**, 51, 275302	3	80
250	The effect of solutes on the precipitate/matrix interface properties in the Vanadium alloys: A first-principles study. *Computational Materials Science*, **2018**, 153, 113-118	3.2	3
249	Dispersive and covalent interactions in all-carbon heterostructures consisting of penta-graphene and fullerene: topological effect. *Journal Physics D: Applied Physics*, **2018**, 51, 305301	3	10
248	Molecular dynamics simulation of wetting behaviors of Li on W surfaces. *Fusion Engineering and Design*, **2017**, 117, 188-193	1.7	8
247	The effects of interstitial impurities on the mechanical properties of vanadium alloys: A first-principles study. *Journal of Alloys and Compounds*, **2017**, 701, 975-980	5.7	11
246	Simultaneous covalent and noncovalent carbon nanotube/AgPO hybrids: new insights into the origin of enhanced visible light photocatalytic performance. *Physical Chemistry Chemical Physics*, **2017**, 19, 7955-7963	3.6	11

245	Construction of g-C 3 N 4 /CeO 2 /ZnO ternary photocatalysts with enhanced photocatalytic performance. *Journal of Physics and Chemistry of Solids*, **2017**, 106, 1-9	3.9	83
244	Hybrid TiO2/graphene derivatives nanocomposites: is functionalized graphene better than pristine graphene for enhanced photocatalytic activity?. *Catalysis Science and Technology*, **2017**, 7, 1423-1432	5.5	17
243	Atomic simulations for configurations and solid-liquid interface of Li-Fe and Li-Cu icosahedra. *Journal of Nanoparticle Research*, **2017**, 19, 1	2.3	3
242	A molecular dynamics study of the transport properties of LiF-BeF 2 -ThF 4 molten salt. *Journal of Molecular Liquids*, **2017**, 234, 220-226	6	7
241	Atomistic simulation of crack propagation in single crystal tungsten under cyclic loading. *Journal of Materials Research*, **2017**, 32, 1474-1483	2.5	6
240	Atomistic simulations of solidification process in B2-LiPb solid(0 0 1)-liquid system. *Journal of Crystal Growth*, **2017**, 470, 113-121	1.6	3
239	Molecular dynamics simulations of the structure evolutions of Cu-Zr metallic glasses under irradiation. *Nuclear Instruments & Methods in Physics Research B*, **2017**, 393, 77-81	1.2	7
238	Investigation of the shock-induced chemical reaction (SICR) in Ni + Al nanoparticle mixtures. *Physical Chemistry Chemical Physics*, **2017**, 19, 17607-17617	3.6	14
237	Non-equilibrium molecular dynamics simulations of the spallation in Ni: Effect of vacancies. *Computational Materials Science*, **2017**, 137, 273-281	3.2	12
236	Two-Dimensional MoS2-Graphene-Based Multilayer van der Waals Heterostructures: Enhanced Charge Transfer and Optical Absorption, and Electric-Field Tunable Dirac Point and Band Gap. *Chemistry of Materials*, **2017**, 29, 5504-5512	9.6	99
235	First-principles study of the adsorption properties of atoms and molecules on UN2 (001) surface. *Journal of Nuclear Materials*, **2017**, 493, 124-131	3.3	1
234	Temperature effects on growth configurations for Al-Mg bimetallic nanoparticles. *Thin Solid Films*, **2017**, 626, 178-183	2.2	2
233	Interfacial interaction in monolayer transition metal dichalcogenide/metal oxide heterostructures and its effects on electronic and optical properties: The case of MX2/CeO2. *Applied Physics Express*, **2017**, 10, 011201	2.4	9
232	Simulation of radiation damages in molybdenum by combining molecular dynamics and OKMC. *Nuclear Science and Techniques/Hewuli*, **2017**, 28, 1	2.1	3
231	Role of electrodes materials in determining the interfacial and magnetoelectric properties in BaTiO3-based multiferroic tunnel junctions. *European Physical Journal B*, **2017**, 90, 1	1.2	14
230	Composition and Size Dependence of Alloying in Ni□Al Nanoparticles With Icosahedral and Rhombohedral Configurations: An Atomic Simulation Study. *Physica Status Solidi (B): Basic Research*, **2017**, 254, 1700168	1.3	
229	Noncovalent Functionalization of Monolayer MoS2 with Carbon Nanotubes: Tuning Electronic Structure and Photocatalytic Activity. *Journal of Physical Chemistry C*, **2017**, 121, 21921-21929	3.8	19
228	The mechanism of enhanced photocatalytic activity of SnO2 through fullerene modification. *Current Applied Physics*, **2017**, 17, 1547-1556	2.6	11

227	Diffusion of Al dimers on the surface of Mg clusters. *European Physical Journal B*, **2017**, 90, 1	1.2	1
226	Phase transition of iron-based single crystals under ramp compressions with extreme strain rates. *International Journal of Plasticity*, **2017**, 96, 56-80	7.6	19
225	Molecular dynamics simulation of diffusion and viscosity of liquid lithium fluoride. *Computational Materials Science*, **2016**, 111, 203-208	3.2	17
224	Dual functions of 2D WS2and MoS2WS2monolayers coupled with a Ag3PO4photocatalyst. *Semiconductor Science and Technology*, **2016**, 31, 095013	1.8	5
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