Chun-Wei Pao

List of Publications by Year
in descending order

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67 papers	1,753 citations	293460 24 h-index	325983 40 g-index
68 all docs	68 docs citations	68 times ranked	3248 citing authors

#	Article	IF	Citations
1	Few-layer fluorine-functionalized graphene hole-selective contacts for efficient inverted perovskite solar cells. Chemical Engineering Journal, 2022, 430, 132831.	6.6	13
2	A highly distorted ultraelastic chemically complex Elinvar alloy. Nature, 2022, 602, 251-257.	13.7	75
3	Improving Thermal and Photostability of Polymer Solar Cells by Robust Interface Engineering. Small, 2022, 18, e2107834.	5.2	8
4	Surface structures and equilibrium shapes of layered 2D Ruddlesden-Popper perovskite crystals from density functional theory calculations. Materials Today Communications, 2021, 26, 101745.	0.9	5
5	Phase-field study of dendritic morphology in lithium metal batteries. Journal of Power Sources, 2021, 484, 229203.	4.0	26
6	Microstructure Maps of Complex Perovskite Materials from Extensive Monte Carlo Sampling Using Machine Learning Enabled Energy Model. Journal of Physical Chemistry Letters, 2021, 12, 3591-3599.	2.1	16
7	An Efficient and Reversible Battery Anode Electrode Derived from a Lead-Based Metalâ€“Organic Framework. Energy & Fuels, 2021, 35, 9669-9682.	2.5	13
8	Structural and Electronic Properties of Intertwined Defect in Ruddlesdenâ€“Popper 2D Perovskites Study Using Density Functional Theory Calculations. Multiscale Science and Engineering, 2021, 3, 205.	0.9	0
9	Understanding chemical short-range ordering/demixing coupled with lattice distortion in solid solution high entropy alloys. Acta Materialia, 2021, 216, 117140.	3.8	52
10	Molecular Simulations of the Microstructure Evolution of Solid Electrolyte Interphase during Cyclic Charging/Discharging. ACS Applied Materials & Interfaces, 2021, 13, 5017-5027.	4.0	10
11	Selfâ€Assembly Behavior of Diacetylenic Acid Molecules upon Vapor Deposition: Oddâ€“Even Effect on the Film Morphology. Chemistry - A European Journal, 2020, 26, 13948-13956.	1.7	4
12	Atomistic Structures and Energetics of Perovskite Nucleation Pathway During Sequential Deposition Process. Multiscale Science and Engineering, 2020, 2, 227-234.	0.9	1
13	Modulating Performance and Stability of Inorganic Lead-Free Perovskite Solar Cells via Lewis-Pair Mediation. ACS Applied Materials & Interfaces, 2020, 12, 32649-32657.	4.0	32
14	Long-lifespan lithiumâ€“metal batteries obtained using a perovskite intercalation layer to stabilize the lithium electrode. Journal of Materials Chemistry A, 2020, 8, 9137-9145.	5.2	4
15	Suppression of surface defects to achieve hysteresis-free inverted perovskite solar cells via quantum dot passivation. Journal of Materials Chemistry A, 2020, 8, 5263-5274.	5.2	67
16	Multiscale molecular simulations of the morphological evolution of small-molecule organic solar cells during the vacuum codeposition process. Physical Review Materials, 2020, 4, .	0.9	0
17	Fast and Accurate Artificial Neural Network Potential Model for MAPbI₃ Perovskite Materials. ACS Omega, 2019, 4, 10950-10959.	1.6	31
18	Multi-layer elemental 2D materials: antimonene, germanene and stanene grown directly on molybdenum disulfides. Semiconductor Science and Technology, 2019, 34, 105020.	1.0	19

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19	A lithium passivated MoO₃ nanobelt decorated polypropylene separator for fast-charging long-life Liâ€“S batteries. Nanoscale, 2019, 11, 2892-2900.	2.8	38
20	ZnO/Silicon-Rich Oxide Superlattices with High Thermoelectric Figure of Merit: A Comprehensive Study by Experiment and Molecular Dynamic Simulation. ACS Applied Materials & Interfaces, 2019, 11, 13507-13513.	4.0	4
21	Artificial Neural Network Model for Atomistic Simulations of $${m {Sb/MoS}_{2}}$$ Sb / MoS 2 van der Waals Heterostructures. Multiscale Science and Engineering, 2019, 1, 119-129.	0.9	9
22	Al-Doped ZnO/Silicon-rich Oxide Superlattices with High Room-Temperature Thermoelectric Figure of Merit. Materials Letters, 2019, 245, 33-36.	1.3	4
23	Mitigating Metal Dendrite Formation in Lithiumâ€“Sulfur Batteries via Morphology-Tunable Graphene Oxide Interfaces. ACS Applied Materials & Interfaces, 2019, 11, 2060-2070.	4.0	19
24	Surface/Interface Stress and Thin Film Stress. , 2019, , 33-55.		0
25	Single-Crystal Antimonene Films Prepared by Molecular Beam Epitaxy: Selective Growth and Contact Resistance Reduction of the 2D Material Heterostructure. ACS Applied Materials & Interfaces, 2018, 10, 15058-15064.	4.0	43
26	Surface/Interface Stress and Thin Film Stress. , 2018, , 1-23.		0
27	Defect formation and modulation during patterning supported graphene sheets using focused ion beams. Materials Today Communications, 2018, 17, 60-68.	0.9	8
28	Folding Sheets with Ion Beams. Nano Letters, 2017, 17, 249-254.	4.5	21
29	Revealing Ordered Polymer Packing during Freeze-Drying Fabrication of a Bulk Heterojunction Poly(3-hexylthiophene-2,5-diyl):[6,6]-Phenyl-C61-butyric Acid Methyl Ester Layer: In Situ Optical Spectroscopy, Molecular Dynamics Simulation, and X-ray Diffraction. Journal of Physical Chemistry C, 2017, 121, 14826-14834.	1.5	7
30	Electronic and carrier transport properties of small molecule donors. Coupled Systems Mechanics, 2017, 6, 75-96.	0.4	0
31	Multiscale Molecular Simulation of Solution Processing of SMDPPEH: PCBM Small-Molecule Organic Solar Cells. ACS Applied Materials & Interfaces, 2016, 8, 20691-20700.	4.0	18
32	Thermoelectric Efficiency of Single-Molecule Junctions: Phase Diagram Constructed from First-Principles Calculations. Journal of Physical Chemistry C, 2015, 119, 28728-28736.	1.5	7
33	PSIIâ€“LHCII Supercomplex Organizations in Photosynthetic Membrane by Coarse-Grained Simulation. Journal of Physical Chemistry B, 2015, 119, 3999-4008.	1.2	15
34	Transferring-free and large-area graphitic carbon film growth by using molecular beam epitaxy at low growth temperature. Journal of Crystal Growth, 2015, 425, 177-180.	0.7	1
35	Anisotropic thermal conductivity of MoS₂ nanoribbons: Chirality and edge effects. Applied Physics Letters, 2014, 104, 201909.	1.5	41
36	Anomalous thermal transport along the grain boundaries of bicrystalline graphene nanoribbons from atomistic simulations. Carbon, 2014, 73, 432-442.	5.4	26

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37	Electrode Materials, Thermal Annealing Sequences, and Lateral/Vertical Phase Separation of Polymer Solar Cells from Multiscale Molecular Simulations. ACS Applied Materials & Interfaces, 2014, 6, 20612-20624.	4.0	27
38	Morphology, molecular stacking, dynamics and device performance correlations of vacuum-deposited small-molecule organic solar cells. Physical Chemistry Chemical Physics, 2014, 16, 8852-8864.	1.3	23
39	Nanomorphology Evolution of P3HT/PCBM Blends during Solution-Processing from Coarse-Grained Molecular Simulations. Journal of Physical Chemistry C, 2014, 118, 11224-11233.	1.5	59
40	Mechanical mutability of polycrystalline graphene from atomistic simulations. Computational Materials Science, 2014, 91, 56-61.	1.4	4
41	Thermal response of grain boundaries in graphene sheets under shear strain from atomistic simulations. Computational Materials Science, 2013, 70, 163-170.	1.4	22
42	2-Alkyl-5-thienyl-Substituted Benzo[1,2-b:4,5-bâ€²]dithiophene-Based Donor Molecules for Solution-Processed Organic Solar Cells. ACS Applied Materials & Interfaces, 2013, 5, 9494-9500.	4.0	70
43	Correlation of nanoscale organizations of polymer and nanocrystals in polymer/inorganic nanocrystal bulk heterojunction hybrid solar cells: insights from multiscale molecular simulations. Energy and Environmental Science, 2013, 6, 307-315.	15.6	16
44	In-situ transmission electron microscopy and first-principles study of Au (100) surface dislocation dynamics. Surface Science, 2013, 608, 154-164.	0.8	5
45	An analytical model for calculating thermal properties of two-dimensional nanomaterials. Applied Physics Letters, 2013, 103, 171909.	1.5	2
46	The formation mechanisms and optical characteristics of GaSb quantum rings. Journal of Applied Physics, 2013, 114, .	1.1	8
47	Low-temperature grown graphene films by using molecular beam epitaxy. Applied Physics Letters, 2012, 101, .	1.5	28
48	Diffusion of the vacancy defect leading to the formation of multi-shell structures in the nanowire and nanobridge. Journal of Applied Physics, 2012, 112, 114301.	1.1	0
49	Dependence of Nanocrystal Dimensionality on the Polymer Nanomorphology, Anisotropic Optical Absorption, and Carrier Transport in P3HT:TiO₂ Bulk Heterojunctions. Journal of Physical Chemistry C, 2012, 116, 25081-25088.	1.5	10
50	Helical multi-shell structures in gold nanobridge and suspending nanowire. Journal of Nanoparticle Research, 2012, 14, 1.	0.8	0
51	Solubility of [6,6]-Phenyl-C₆₁-butyric Acid Methyl Ester and Optimal Blending Ratio of Bulk Heterojunction Polymer Solar Cells. Journal of Physical Chemistry C, 2012, 116, 12455-12461.	1.5	33
52	Decoupling of CVD graphene by controlled oxidation of recrystallized Cu. RSC Advances, 2012, 2, 3008.	1.7	82
53	Graphene defect polarity dynamics. Carbon, 2012, 50, 2870-2876.	5.4	21
54	Effects of dislocation densities and distributions on graphene grain boundary failure strengths from atomistic simulations. Carbon, 2012, 50, 3465-3472.	5.4	86

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55	Ab initio calculations of the reaction pathways for methane decomposition over the Cu (111) surface. Journal of Chemical Physics, 2011, 135, 064707.	1.2	78
56	Multiscale molecular simulations of the nanoscale morphologies of P3HT:PCBM blends for bulk heterojunction organic photovoltaic cells. Energy and Environmental Science, 2011, 4, 4124.	15.6	122
57	Structure, energy, and structural transformations of graphene grain boundaries from atomistic simulations. Carbon, 2011, 49, 2306-2317.	5.4	137
58	Atomistic simulations of stress and microstructure evolution during polycrystalline Ni film growth. Physical Review B, 2009, 79, .	1.1	32
59	Compressive film stress in a thin, tensile heteroepitaxial film. Applied Physics Letters, 2008, 93, 011903.	1.5	2
60	Thermodynamic and kinetic properties of surface dislocations on Au(001) from atomistic simulations. Physical Review B, 2007, 75, .	1.1	5
61	Thin Film Compressive Stresses due to Adatom Insertion into Grain Boundaries. Physical Review Letters, 2007, 99, 036102.	2.9	82
62	Dislocation Injection, Reconstruction, and Atomic Transport on {001} Au Terraces. Physical Review Letters, 2007, 98, 036103.	2.9	17
63	Stress and Morphology Evolution during Island Growth. Physical Review Letters, 2006, 96, 186103.	2.9	47
64	Atomistic simulation of stress evolution during island growth. Journal of the Mechanics and Physics of Solids, 2006, 54, 2527-2543.	2.3	19
65	Comparison of the electronic structures of Zn1â^'xCoxO and Zn1â^'xMgxO nanorods using x-ray absorption and scanning photoelectron microscopies. Applied Physics Letters, 2006, 89, 043121.	1.5	35
66	Effects of surface defects on surface stress of Cu(001) and Cu(111). Physical Review B, 2006, 74, .	1.1	33
67	Bonding properties and their relation to residual stress and refractive index of amorphous Ta(N,O) films investigated by x-ray absorption spectroscopy. Applied Physics Letters, 2005, 86, 161910.	1.5	10