Paulette Clancy

List of Publications by Year
in descending order

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81	2,291	361045	223531
papers	citations	20 h-index	46 g-index

81	81	81	3838
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Pentacene Thin Film Growth. Chemistry of Materials, 2004, 16, 4497-4508.	3.2	588
2	Understanding Polymorphism in Organic Semiconductor Thin Films through Nanoconfinement. Journal of the American Chemical Society, 2014, 136, 17046-17057.	6.6	179
3	One-dimensional self-confinement promotes polymorph selection in large-area organic semiconductor thin films. Nature Communications, 2014, 5, 3573.	5.8	129
4	Controlling nucleation, growth, and orientation of metal halide perovskite thin films with rationally selected additives. Journal of Materials Chemistry A, 2017, 5, 113-123.	5.2	115
5	Mayer Bond Order as a Metric of Complexation Effectiveness in Lead Halide Perovskite Solutions. Chemistry of Materials, 2017, 29, 2435-2444.	3.2	82
6	Efficient search of compositional space for hybrid organicâ€“inorganic perovskites via Bayesian optimization. Npj Computational Materials, 2018, 4, .	3.5	82
7	A classification scheme for the stacking of two-dimensional boronate ester-linked covalent organic frameworks. Journal of Materials Chemistry, 2012, 22, 17460.	6.7	73
8	Metalâ€“Organic Framework-Inspired Metal-Containing Clusters for High-Resolution Patterning. Chemistry of Materials, 2018, 30, 4124-4133.	3.2	65
9	Membrane alternatives in worlds without oxygen: Creation of an azotosome. Science Advances, 2015, 1, e1400067.	4.7	61
10	Highly Efficient Benzannulation of Poly(phenylene ethynylene)s. Angewandte Chemie - International Edition, 2012, 51, 12051-12054.	7.2	55
11	Halogenation of a Nonplanar Molecular Semiconductor to Tune Energy Levels and Bandgaps for Electron Transport. Chemistry of Materials, 2015, 27, 1892-1900.	3.2	55
12	Application of Molecular Simulation Techniques to the Study of Factors Affecting the Thin-Film Morphology of Small-Molecule Organic Semiconductors. Chemistry of Materials, 2011, 23, 522-543.	3.2	52
13	Ambipolar Transport in Solution-Synthesized Graphene Nanoribbons. ACS Nano, 2016, 10, 4847-4856.	7.3	52
14	Equilibrium concentrations of defects in pure and Bâ€doped silicon. Journal of Applied Physics, 1996, 79, 8998-9011.	1.1	46
15	Sulfur-Donor Solvents Strongly Coordinate Pb²⁺ in Hybrid Organicâ€“Inorganic Perovskite Precursor Solutions. Journal of Physical Chemistry C, 2020, 124, 14496-14502.	1.5	38
16	The Role of Shape on Electronic Structure and Charge Transport in Faceted PbSe Nanocrystals. ACS Nano, 2014, 8, 2302-2317.	7.3	31
17	Computational Implementation of Nudged Elastic Band, Rigid Rotation, and Corresponding Force Optimization. Journal of Chemical Theory and Computation, 2017, 13, 3250-3259.	2.3	29
18	Exploring the Energetic Deposition of Pentacene on Pentacene through Molecular Dynamics Simulationsâ€. Journal of Physical Chemistry C, 2007, 111, 15653-15659.	1.5	28

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19	Using Preformed Meisenheimer Complexes as Dopants for nâ€Type Organic Thermoelectrics with High Seebeck Coefficients and Power Factors. Advanced Functional Materials, 2021, 31, 2010567.	7.8	28
20	Single Atom Substitution Alters the Polymorphic Transition Mechanism in Organic Electronic Crystals. Chemistry of Materials, 2019, 31, 9115-9126.	3.2	27
21	Theoretical Investigation of Charge-Transfer Processes at Pentaceneâ€“C60 Interface: The Importance of Triplet Charge Separation and Marcus Electron Transfer Theory. Journal of Physical Chemistry C, 2014, 118, 23605-23613.	1.5	20
22	3,4,5â€Trimethoxy Substitution on an Nâ€DMBI Dopant with New Nâ€Type Polymers: Polymerâ€Dopant Matching for Improved Conductivityâ€Seebeck Coefficient Relationship. Angewandte Chemie - International Edition, 2021, 60, 27212-27219.	7.2	20
23	Experimental determination of thermal profiles during laser spike annealing with quantitative comparison to 3-dimensional simulations. Applied Physics Letters, 2012, 100, .	1.5	19
24	The efficacy of Lewis affinity scale metrics to represent solvent interactions with reagent salts in all-inorganic metal halide perovskite solutions. Journal of Materials Chemistry A, 2021, 9, 13087-13099.	5.2	19
25	Solvation of nitrogen compounds in Titanâ€™s seas, precipitates, and atmosphere. Icarus, 2015, 256, 1-12.	1.1	18
26	Finite element and analytical solutions for van der Pauw and four-point probe correction factors when multiple non-ideal measurement conditions coexist. Review of Scientific Instruments, 2017, 88, 094704.	0.6	18
27	Deactivation kinetics of supersaturated boron:silicon alloys. Journal of Applied Physics, 2001, 90, 2262-2268.	1.1	16
28	Cost-effective materials discovery: Bayesian optimization across multiple information sources. Materials Horizons, 2020, 7, 2113-2123.	6.4	15
29	Molecular-Scale Events in Hyperthermal Deposition of Organic Semiconductors Implicated from Experiment and Molecular Simulation. Journal of Physical Chemistry C, 2009, 113, 6068-6073.	1.5	14
30	Pentacene-based nanorods on Au(111) single crystals: Charge transfer, diffusion, and step-edge barriers. Nano Research, 2013, 6, 449-459.	5.8	14
31	Connecting the Particles in the Box - Controlled Fusion of Hexamer Nanocrystal Clusters within an AB6 Binary Nanocrystal Superlattice. Scientific Reports, 2014, 4, 6731.	1.6	13
32	Multiscale Simulation and Modeling of Multilayer Heteroepitactic Growth of C₆₀ on Pentacene. Langmuir, 2016, 32, 3045-3056.	1.6	13
33	Bypassing Solid-State Intermediates by Solvent Engineering the Crystallization Pathway in Hybrid Organicâ€“Inorganic Perovskites. Crystal Growth and Design, 2020, 20, 1162-1171.	1.4	13
34	Synthesis and Solution-Phase Characterization of Sulfonated Oligothioetheramides. Macromolecules, 2017, 50, 8731-8738.	2.2	12
35	Classification of spatially resolved molecular fingerprints for machine learning applications and development of a codebase for their implementation. Molecular Systems Design and Engineering, 2018, 3, 431-441.	1.7	12
36	Stochastic Fusion Simulations and Experiments Suggest Passive and Active Roles of Hemagglutinin during Membrane Fusion. Biophysical Journal, 2014, 106, 843-854.	0.2	11

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37	A Kinetic Monte Carlo Study of Fullerene Adsorption within a Pc-PBBA Covalent Organic Framework and Implications for Electron Transport. Journal of Chemical Theory and Computation, 2015, 11, 1172-1180.	2.3	11
38	Energetics of neutral Si dopants in InGaAs: Anab initioand semiempirical Tersoff model study. Physical Review B, 2015, 91, .	1.1	11
39	Modeling the thermal poling of glasses using molecular dynamics. Part 1: Effects on glass structure. Journal of Non-Crystalline Solids, 2017, 461, 98-103.	1.5	11
40	A New Kinetic Monte Carlo Algorithm for Heteroepitactical Growth: Case Study of C₆₀ Growth on Pentacene. Journal of Chemical Theory and Computation, 2012, 8, 1048-1057.	2.3	10
41	How well do implicit solvation models represent intermolecular binding energies in organic-inorganic solutions?. Computational Materials Science, 2019, 170, 109138.	1.4	10
42	A new metric to control nucleation and grain size distribution in hybrid organicâ€“inorganic perovskites by tuning the dielectric constant of the antisolvent. Journal of Materials Chemistry A, 2021, 9, 3668-3676.	5.2	10
43	Ab initio modeling of vacancies, antisites, and Si dopants in ordered InGaAs. Journal of Applied Physics, 2017, 121, .	1.1	9
44	Uncovering the reaction mechanism initiating the nucleation of lead sulfide quantum dots in a hines synthesis. Journal of Materials Chemistry A, 2018, 6, 9402-9410.	5.2	9
45	A Quantitative Metric for the Design of Selective Supercritical CO₂ Extraction of Lithium from Geothermal Brine. ChemSusChem, 2019, 12, 3532-3540.	3.6	9
46	The Role of Dimer Formation in the Nucleation of Superlattice Transformations and Its Impact on Disorder. ACS Nano, 2020, 14, 11431-11441.	7.3	9
47	Effect of edge-functionalization on the ease of graphene nanoribbon aggregation in solvent. Carbon, 2017, 115, 154-161.	5.4	8
48	Protocol for Directing Nudged Elastic Band Calculations to the Minimum Energy Pathway: Nurturing Errant Calculations Back to Convergence. Journal of Chemical Theory and Computation, 2022, 18, 2993-3005.	2.3	8
49	A molecular dynamics study of the effect of pentacene polymorphs on C60surface adsorption and diffusional properties and the tendency to form nanowires. Molecular Simulation, 2010, 36, 590-603.	0.9	7
50	Chemical engineering in the electronics industry: progress towards the rational design of organic semiconductor heterojunctions. Current Opinion in Chemical Engineering, 2012, 1, 117-122.	3.8	7
51	Simulation of Graphene Nanoribbon Aggregation and Its Mediation by Edge Decoration. Journal of Physical Chemistry B, 2015, 119, 4766-4776.	1.2	7
52	Towards optimal packing and diffusion of fullerene molecules in the Pc-PBBA covalent organic framework. Molecular Simulation, 2014, 40, 58-70.	0.9	6
53	Factors affecting tacticity and aggregation of P3HT polymers in P3HT:PCBM blends. Molecular Simulation, 2017, 43, 743-755.	0.9	6
54	Solventâ€“Molecule Interactions Govern Crystal-Habit Selection in Naphthalene Tetracarboxylic Diimides. Chemistry of Materials, 2019, 31, 9691-9698.	3.2	6

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55	Decomplexation as a rate limitation in the thiol-Michael addition of N-acrylamides. Organic and Biomolecular Chemistry, 2020, 18, 6364-6377.	1.5	6
56	Direct melt processing of pentacene at temperatures above 1000â€‰Â°C by pulsed laser irradiation. Applied Physics Letters, 2008, 93, .	1.5	5
57	Parameter-free correlation for a composition-based prediction of the dielectric constant of amorphous organosilicate materials. Molecular Simulation, 2012, 38, 1221-1233.	0.9	5
58	Structural characterization of amorphous materials applied to low-k organosilicate materials. Thin Solid Films, 2014, 562, 411-422.	0.8	5
59	Effect of Laser Annealing on the Structure of Amorphous Porous SiCOH Materials. Journal of Physical Chemistry C, 2015, 119, 12616-12624.	1.5	5
60	Ab Initio Studies of the Diffusion of Intrinsic Defects and Silicon Dopants in Bulk InAs. Langmuir, 2017, 33, 11484-11489.	1.6	5
61	Preferred diffusional pathways of intrinsic defects and silicon dopants in an ordered phase of In0.5Ga0.5As: A first-principles study. Acta Materialia, 2017, 140, 39-45.	3.8	5
62	Transferable Molecular Model of Woven Covalent Organic Framework Materials. ACS Applied Materials & Interfaces, 2020, 12, 48957-48968.	4.0	4
63	Balancing Multiple Goals and Making It Work for Materials Research. ACS Central Science, 2020, 6, 464-466.	5.3	4
64	Ab Initio modeling of Near-Edge EELS spectra for chemisorbed molecules. Nanotechnology, 2021, 32, 355702.	1.3	4
65	Untying the Cesium â€œNotâ€• Cesiumâ€“Iodoplumbate Complexation in Perovskite Solution-Processing Inks Has Implications for Crystallization. Journal of Physical Chemistry Letters, 2022, 13, 6130-6137.	2.1	4
66	Organic Heterojunctions for Photovoltaic Applications: C60 Growth on Pentacene. Materials Research Society Symposia Proceedings, 2010, 1263, 50601.	0.1	3
67	A 3D model for simulating temperature and stress profiles during sub-millisecond laser spike annealing. , 2010, , .		3
68	Modeling the thermal poling of glasses using molecular dynamics. Part 2: Effects on elastic properties. Journal of Non-Crystalline Solids, 2017, 468, 17-26.	1.5	3
69	Density functional theory studies of reaction mechanisms for titanium alkylamide incorporation onto functionalized aromatic self-assembled monolayers. Journal of Materials Chemistry, 2007, 17, 3927.	6.7	2
70	Simple Molecular Reactive Force Field for Metalâ€“Organic Synthesis. Journal of Chemical Theory and Computation, 2016, 12, 825-838.	2.3	2
71	Contorted Octabenzocircumbiphenyl Sorts Semiconducting Single-Walled Carbon Nanotubes with Structural Specificity. Chemistry of Materials, 2017, 29, 595-604.	3.2	2
72	Resolving the mystery of the concentration-dependence of amphoteric dopant diffusion in III-V semiconductors. Acta Materialia, 2020, 186, 555-563.	3.8	2

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73	Evidence of Preformed Lewis Acidâ€“Base and Wheland-Type Complexes Acting as Dopants for p-Type Conjugated Polymers. ACS Applied Polymer Materials, 2022, 4, 2065-2080.	2.0	2
74	A feasibility study of unconventional planar ligand spacers in chalcogenide nanocrystals. Physical Chemistry Chemical Physics, 2016, 18, 13781-13793.	1.3	1
75	Fingerprinting the vibrational signatures of dopants and defects in a fully random alloy: An ab initio case study of Si, Se, and vacancies in In0.5Ga0.5As. Journal of Applied Physics, 2020, 127, 205704.	1.1	1
76	3,4,5â€Trimethoxy Substitution on an Nâ€DMBI Dopant with New Nâ€Type Polymers: Polymerâ€Dopant Matching for Improved Conductivityâ€Seebeck Coefficient Relationship. Angewandte Chemie, 2021, 133, 27418-27425.	1.6	1
77	Preferred Interfacial Alignment in the Pd@HKUST1 System and the Role of the MOF to Affect Charge Transfer to Pd Nanoparticles. Journal of Physical Chemistry C, 2022, 126, 11709-11714.	1.5	1
78	Dissolution and Growth Kinetics of Small Crystals in Liquids. Materials Research Society Symposia Proceedings, 1991, 238, 279.	0.1	0
79	Development of a Suite of Computational Models for the Design of Ultralow-k SiCOH-based Materials. Materials Research Society Symposia Proceedings, 2012, 1428, 45.	0.1	0
80	Prediction of the Interface Response Functions for Amorphous and Crystalline Phases of Silicon and Germanium. Materials Research Society Symposia Proceedings, 2003, 762, 1641.	0.1	0
81	Molecular modeling of interfacial layer-by-layer assembly towards functionalized capsule materials. Nanoscale, 2021, 13, 19915-19928.	2.8	0