Paulette Clancy

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

74 papers	1,824 citations	18 h-index	41 g-index
81 ext. papers	2,053 ext. citations	7.2 avg, IF	4.8 L-index

#	Paper	IF	Citations
74	Evidence of Preformed Lewis Acid–Base and Wheland-Type Complexes Acting as Dopants for p-Type Conjugated Polymers. *ACS Applied Polymer Materials*, **2022**, 4, 2065-2080	4.3	1
73	3,4,5-Trimethoxy Substitution on an N-DMBI Dopant with New N-Type Polymers: Polymer-Dopant Matching for Improved Conductivity-Seebeck Coefficient Relationship. *Angewandte Chemie - International Edition*, **2021**, 60, 27212	16.4	8
72	Using Preformed Meisenheimer Complexes as Dopants for n-Type Organic Thermoelectrics with High Seebeck Coefficients and Power Factors. *Advanced Functional Materials*, **2021**, 31, 2010567	15.6	17
71	A new metric to control nucleation and grain size distribution in hybrid organic–inorganic perovskites by tuning the dielectric constant of the antisolvent. *Journal of Materials Chemistry A*, **2021**, 9, 3668-3676	13	3
70	Sulfur-Donor Solvents Strongly Coordinate Pb2+ in Hybrid Organic–Inorganic Perovskite Precursor Solutions. *Journal of Physical Chemistry C*, **2020**, 124, 14496-14502	3.8	21
69	Cost-effective materials discovery: Bayesian optimization across multiple information sources. *Materials Horizons*, **2020**, 7, 2113-2123	14.4	10
68	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	2.5	0
67	Bypassing Solid-State Intermediates by Solvent Engineering the Crystallization Pathway in Hybrid Organic–Inorganic Perovskites. *Crystal Growth and Design*, **2020**, 20, 1162-1171	3.5	6
66	Resolving the mystery of the concentration-dependence of amphoteric dopant diffusion in III-V semiconductors. *Acta Materialia*, **2020**, 186, 555-563	8.4	
65	Transferable Molecular Model of Woven Covalent Organic Framework Materials. *ACS Applied Materials & Interfaces*, **2020**, 12, 48957-48968	9.5	2
64	Decomplexation as a rate limitation in the thiol-Michael addition of N-acrylamides. *Organic and Biomolecular Chemistry*, **2020**, 18, 6364-6377	3.9	3
63	The Role of Dimer Formation in the Nucleation of Superlattice Transformations and Its Impact on Disorder. *ACS Nano*, **2020**, 14, 11431-11441	16.7	4
62	How well do implicit solvation models represent intermolecular binding energies in organic-inorganic solutions?. *Computational Materials Science*, **2019**, 170, 109138	3.2	5
61	A Quantitative Metric for the Design of Selective Supercritical CO Extraction of Lithium from Geothermal Brine. *ChemSusChem*, **2019**, 12, 3532-3540	8.3	6
60	Single Atom Substitution Alters the Polymorphic Transition Mechanism in Organic Electronic Crystals. *Chemistry of Materials*, **2019**, 31, 9115-9126	9.6	16
59	Solvent–Molecule Interactions Govern Crystal-Habit Selection in Naphthalene Tetracarboxylic Diimides. *Chemistry of Materials*, **2019**, 31, 9691-9698	9.6	3
58	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	4.6	11

57	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	13	7
56	Metal□Organic Framework-Inspired Metal-Containing Clusters for High-Resolution Patterning. *Chemistry of Materials*, **2018**, 30, 4124-4133	9.6	29
55	Efficient search of compositional space for hybrid organic□inorganic perovskites via Bayesian optimization. *Npj Computational Materials*, **2018**, 4,	10.9	49
54	Contorted Octabenzocircumbiphenyl Sorts Semiconducting Single-Walled Carbon Nanotubes with Structural Specificity. *Chemistry of Materials*, **2017**, 29, 595-604	9.6	1
53	Effect of edge-functionalization on the ease of graphene nanoribbon aggregation in solvent. *Carbon*, **2017**, 115, 154-161	10.4	8
52	Modeling the thermal poling of glasses using molecular dynamics. Part 1: Effects on glass structure. *Journal of Non-Crystalline Solids*, **2017**, 461, 98-103	3.9	9
51	Modeling the thermal poling of glasses using molecular dynamics. Part 2: Effects on elastic properties. *Journal of Non-Crystalline Solids*, **2017**, 468, 17-26	3.9	1
50	Computational Implementation of Nudged Elastic Band, Rigid Rotation, and Corresponding Force Optimization. *Journal of Chemical Theory and Computation*, **2017**, 13, 3250-3259	6.4	17
49	Factors affecting tacticity and aggregation of P3HT polymers in P3HT:PCBM blends. *Molecular Simulation*, **2017**, 43, 743-755	2	4
48	Ab initio modeling of vacancies, antisites, and Si dopants in ordered InGaAs. *Journal of Applied Physics*, **2017**, 121, 045106	2.5	7
47	Mayer Bond Order as a Metric of Complexation Effectiveness in Lead Halide Perovskite Solutions. *Chemistry of Materials*, **2017**, 29, 2435-2444	9.6	52
46	Ab Initio Studies of the Diffusion of Intrinsic Defects and Silicon Dopants in Bulk InAs. *Langmuir*, **2017**, 33, 11484-11489	4	3
45	Synthesis and Solution-Phase Characterization of Sulfonated Oligothioetheramides. *Macromolecules*, **2017**, 50, 8731-8738	5.5	9
44	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	1.7	8
43	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	8.4	3
42	Controlling nucleation, growth, and orientation of metal halide perovskite thin films with rationally selected additives. *Journal of Materials Chemistry A*, **2017**, 5, 113-123	13	92
41	Simple Molecular Reactive Force Field for Metal-Organic Synthesis. *Journal of Chemical Theory and Computation*, **2016**, 12, 825-38	6.4	1
40	Multiscale Simulation and Modeling of Multilayer Heteroepitactic Growth of C60 on Pentacene. *Langmuir*, **2016**, 32, 3045-56	4	11

39	A feasibility study of unconventional planar ligand spacers in chalcogenide nanocrystals. *Physical Chemistry Chemical Physics*, **2016**, 18, 13781-93	3.6	1
38	Ambipolar Transport in Solution-Synthesized Graphene Nanoribbons. *ACS Nano*, **2016**, 10, 4847-56	16.7	45
37	Solvation of nitrogen compounds in Titan's seas, precipitates, and atmosphere. *Icarus*, **2015**, 256, 1-12	3.8	15
36	Membrane alternatives in worlds without oxygen: Creation of an azotosome. *Science Advances*, **2015**, 1, e1400067	14.3	44
35	Halogenation of a Nonplanar Molecular Semiconductor to Tune Energy Levels and Bandgaps for Electron Transport. *Chemistry of Materials*, **2015**, 27, 1892-1900	9.6	46
34	Energetics of neutral Si dopants in InGaAs: An ab initio and semiempirical Tersoff model study. *Physical Review B*, **2015**, 91,	3.3	10
33	Effect of Laser Annealing on the Structure of Amorphous Porous SiCOH Materials. *Journal of Physical Chemistry C*, **2015**, 119, 12616-12624	3.8	3
32	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, 1172-80	6.4	10
31	Simulation of graphene nanoribbon aggregation and its mediation by edge decoration. *Journal of Physical Chemistry B*, **2015**, 119, 4766-76	3.4	5
30	Connecting the particles in the box--controlled fusion of hexamer nanocrystal clusters within an AB$_{13}$ binary nanocrystal superlattice. *Scientific Reports*, **2014**, 4, 6731	4.9	12
29	Stochastic fusion simulations and experiments suggest passive and active roles of hemagglutinin during membrane fusion. *Biophysical Journal*, **2014**, 106, 843-54	2.9	9
28	Structural characterization of amorphous materials applied to low-k organosilicate materials. *Thin Solid Films*, **2014**, 562, 411-422	2.2	5
27	One-dimensional self-confinement promotes polymorph selection in large-area organic semiconductor thin films. *Nature Communications*, **2014**, 5, 3573	17.4	116
26	Towards optimal packing and diffusion of fullerene molecules in the Pc-PBBA covalent organic framework. *Molecular Simulation*, **2014**, 40, 58-70	2	6
25	Theoretical Investigation of Charge-Transfer Processes at Pentacene$_{16}$C60 Interface: The Importance of Triplet Charge Separation and Marcus Electron Transfer Theory. *Journal of Physical Chemistry C*, **2014**, 118, 23605-23613	3.8	18
24	The role of shape on electronic structure and charge transport in faceted PbSe nanocrystals. *ACS Nano*, **2014**, 8, 2302-17	16.7	28
23	Understanding polymorphism in organic semiconductor thin films through nanoconfinement. *Journal of the American Chemical Society*, **2014**, 136, 17046-57	16.4	155
22	Pentacene-based nanorods on Au(111) single crystals: Charge transfer, diffusion, and step-edge barriers. *Nano Research*, **2013**, 6, 449-459	10	12

21	Highly efficient benzannulation of poly(phenylene ethynylene)s. *Angewandte Chemie - International Edition*, **2012**, 51, 12051-4	16.4	50
20	Parameter-free correlation for a composition-based prediction of the dielectric constant of amorphous organosilicate materials. *Molecular Simulation*, **2012**, 38, 1221-1233	2	5
19	A New Kinetic Monte Carlo Algorithm for Heteroepitactical Growth: Case Study of C60 Growth on Pentacene. *Journal of Chemical Theory and Computation*, **2012**, 8, 1048-57	6.4	8
18	A classification scheme for the stacking of two-dimensional boronate ester-linked covalent organic frameworks. *Journal of Materials Chemistry*, **2012**, 22, 17460		55
17	Chemical engineering in the electronics industry: progress towards the rational design of organic semiconductor heterojunctions. *Current Opinion in Chemical Engineering*, **2012**, 1, 117-122	5.4	5
16	Development of a Suite of Computational Models for the Design of Ultralow-k SiCOH-based Materials. *Materials Research Society Symposia Proceedings*, **2012**, 1428, 45		
15	Experimental determination of thermal profiles during laser spike annealing with quantitative comparison to 3-dimensional simulations. *Applied Physics Letters*, **2012**, 100, 211915	3.4	18
14	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	9.6	47
13	Organic Heterojunctions for Photovoltaic Applications: C60 Growth on Pentacene. *Materials Research Society Symposia Proceedings*, **2010**, 1263, 50601		3
12	A molecular dynamics study of the effect of pentacene polymorphs on C60 surface adsorption and diffusional properties and the tendency to form nanowires. *Molecular Simulation*, **2010**, 36, 590-603	2	5
11	A 3D model for simulating temperature and stress profiles during sub-millisecond laser spike annealing **2010**,		3
10	Molecular-Scale Events in Hyperthermal Deposition of Organic Semiconductors Implicated from Experiment and Molecular Simulation. *Journal of Physical Chemistry C*, **2009**, 113, 6068-6073	3.8	13
9	Direct melt processing of pentacene at temperatures above 1000 °C by pulsed laser irradiation. *Applied Physics Letters*, **2008**, 93, 183306	3.4	5
8	Exploring the Energetic Deposition of Pentacene on Pentacene through Molecular Dynamics Simulations *Journal of Physical Chemistry C*, **2007**, 111, 15653-15659	3.8	27
7	Density functional theory studies of reaction mechanisms for titanium alkylamide incorporation onto functionalized aromatic self-assembled monolayers. *Journal of Materials Chemistry*, **2007**, 17, 3927		1
6	Pentacene Thin Film Growth. *Chemistry of Materials*, **2004**, 16, 4497-4508	9.6	541
5	Prediction of the Interface Response Functions for Amorphous and Crystalline Phases of Silicon and Germanium. *Materials Research Society Symposia Proceedings*, **2003**, 762, 1641		
4	Deactivation kinetics of supersaturated boron:silicon alloys. *Journal of Applied Physics*, **2001**, 90, 2262-2268	2.5	14

3	Equilibrium concentrations of defects in pure and B-doped silicon. *Journal of Applied Physics*, **1996**, 79, 8998-9011	2.5	44
2	Dissolution and Growth Kinetics of Small Crystals in Liquids. *Materials Research Society Symposia Proceedings*, **1991**, 238, 279		
1	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*,	13	9