

Paulette Clancy

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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	Pentacene Thin Film Growth. <i>Chemistry of Materials</i> , 2004 , 16, 4497-4508	9.6	541
73	Understanding polymorphism in organic semiconductor thin films through nanoconfinement. <i>Journal of the American Chemical Society</i> , 2014 , 136, 17046-57	16.4	155
72	One-dimensional self-confinement promotes polymorph selection in large-area organic semiconductor thin films. <i>Nature Communications</i> , 2014 , 5, 3573	17.4	116
71	Controlling nucleation, growth, and orientation of metal halide perovskite thin films with rationally selected additives. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 113-123	13	92
70	A classification scheme for the stacking of two-dimensional boronate ester-linked covalent organic frameworks. <i>Journal of Materials Chemistry</i> , 2012 , 22, 17460		55
69	Mayer Bond Order as a Metric of Complexation Effectiveness in Lead Halide Perovskite Solutions. <i>Chemistry of Materials</i> , 2017 , 29, 2435-2444	9.6	52
68	Highly efficient benzannulation of poly(phenylene ethynylene)s. <i>Angewandte Chemie - International Edition</i> , 2012 , 51, 12051-4	16.4	50
67	Efficient search of compositional space for hybrid organic-inorganic perovskites via Bayesian optimization. <i>Npj Computational Materials</i> , 2018 , 4,	10.9	49
66	Application of Molecular Simulation Techniques to the Study of Factors Affecting the Thin-Film Morphology of Small-Molecule Organic Semiconductors. <i>Chemistry of Materials</i> , 2011 , 23, 522-543	9.6	47
65	Halogenation of a Nonplanar Molecular Semiconductor to Tune Energy Levels and Bandgaps for Electron Transport. <i>Chemistry of Materials</i> , 2015 , 27, 1892-1900	9.6	46
64	Ambipolar Transport in Solution-Synthesized Graphene Nanoribbons. <i>ACS Nano</i> , 2016 , 10, 4847-56	16.7	45
63	Membrane alternatives in worlds without oxygen: Creation of an azotosome. <i>Science Advances</i> , 2015 , 1, e1400067	14.3	44
62	Equilibrium concentrations of defects in pure and B-doped silicon. <i>Journal of Applied Physics</i> , 1996 , 79, 8998-9011	2.5	44
61	Metal-Organic Framework-Inspired Metal-Containing Clusters for High-Resolution Patterning. <i>Chemistry of Materials</i> , 2018 , 30, 4124-4133	9.6	29
60	The role of shape on electronic structure and charge transport in faceted PbSe nanocrystals. <i>ACS Nano</i> , 2014 , 8, 2302-17	16.7	28
59	Exploring the Energetic Deposition of Pentacene on Pentacene through Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 15653-15659	3.8	27
58	Sulfur-Donor Solvents Strongly Coordinate Pb ²⁺ in Hybrid Organic-Inorganic Perovskite Precursor Solutions. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 14496-14502	3.8	21

57	Theoretical Investigation of Charge-Transfer Processes at Pentacene/C60 Interface: The Importance of Triplet Charge Separation and Marcus Electron Transfer Theory. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 23605-23613	3.8	18
56	Experimental determination of thermal profiles during laser spike annealing with quantitative comparison to 3-dimensional simulations. <i>Applied Physics Letters</i> , 2012 , 100, 211915	3.4	18
55	Computational Implementation of Nudged Elastic Band, Rigid Rotation, and Corresponding Force Optimization. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 3250-3259	6.4	17
54	Using Preformed Meisenheimer Complexes as Dopants for n-Type Organic Thermoelectrics with High Seebeck Coefficients and Power Factors. <i>Advanced Functional Materials</i> , 2021 , 31, 2010567	15.6	17
53	Single Atom Substitution Alters the Polymorphic Transition Mechanism in Organic Electronic Crystals. <i>Chemistry of Materials</i> , 2019 , 31, 9115-9126	9.6	16
52	Solvation of nitrogen compounds in Titanian seas, precipitates, and atmosphere. <i>Icarus</i> , 2015 , 256, 1-12	3.8	15
51	Deactivation kinetics of supersaturated boron:silicon alloys. <i>Journal of Applied Physics</i> , 2001 , 90, 2262-2268	2.6	14
50	Molecular-Scale Events in Hyperthermal Deposition of Organic Semiconductors Implicated from Experiment and Molecular Simulation. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 6068-6073	3.8	13
49	Connecting the particles in the box--controlled fusion of hexamer nanocrystal clusters within an AB binary nanocrystal superlattice. <i>Scientific Reports</i> , 2014 , 4, 6731	4.9	12
48	Pentacene-based nanorods on Au(111) single crystals: Charge transfer, diffusion, and step-edge barriers. <i>Nano Research</i> , 2013 , 6, 449-459	10	12
47	Classification of spatially resolved molecular fingerprints for machine learning applications and development of a codebase for their implementation. <i>Molecular Systems Design and Engineering</i> , 2018 , 3, 431-441	4.6	11
46	Multiscale Simulation and Modeling of Multilayer Heteroepitactic Growth of C60 on Pentacene. <i>Langmuir</i> , 2016 , 32, 3045-56	4	11
45	Energetics of neutral Si dopants in InGaAs: An ab initio and semiempirical Tersoff model study. <i>Physical Review B</i> , 2015 , 91,	3.3	10
44	Cost-effective materials discovery: Bayesian optimization across multiple information sources. <i>Materials Horizons</i> , 2020 , 7, 2113-2123	14.4	10
43	A Kinetic Monte Carlo Study of Fullerene Adsorption within a Pc-PBBA Covalent Organic Framework and Implications for Electron Transport. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 1172-80	6.4	10
42	Modeling the thermal poling of glasses using molecular dynamics. Part 1: Effects on glass structure. <i>Journal of Non-Crystalline Solids</i> , 2017 , 461, 98-103	3.9	9
41	Synthesis and Solution-Phase Characterization of Sulfonated Oligothioetheramides. <i>Macromolecules</i> , 2017 , 50, 8731-8738	5.5	9
40	Stochastic fusion simulations and experiments suggest passive and active roles of hemagglutinin during membrane fusion. <i>Biophysical Journal</i> , 2014 , 106, 843-54	2.9	9

39	The efficacy of Lewis affinity scale metrics to represent solvent interactions with reagent salts in all-inorganic metal halide perovskite solutions. <i>Journal of Materials Chemistry A</i> ,	13	9
38	Effect of edge-functionalization on the ease of graphene nanoribbon aggregation in solvent. <i>Carbon</i> , 2017 , 115, 154-161	10.4	8
37	Finite element and analytical solutions for van der Pauw and four-point probe correction factors when multiple non-ideal measurement conditions coexist. <i>Review of Scientific Instruments</i> , 2017 , 88, 094704	17.04	8
36	A New Kinetic Monte Carlo Algorithm for Heteroepitaxial Growth: Case Study of C60 Growth on Pentacene. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 1048-57	6.4	8
35	3,4,5-Trimethoxy Substitution on an N-DMBI Dopant with New N-Type Polymers: Polymer-Dopant Matching for Improved Conductivity-Seebeck Coefficient Relationship. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 27212	16.4	8
34	Ab initio modeling of vacancies, antisites, and Si dopants in ordered InGaAs. <i>Journal of Applied Physics</i> , 2017 , 121, 045106	2.5	7
33	Uncovering the reaction mechanism initiating the nucleation of lead sulfide quantum dots in a hines synthesis. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 9402-9410	13	7
32	A Quantitative Metric for the Design of Selective Supercritical CO Extraction of Lithium from Geothermal Brine. <i>ChemSusChem</i> , 2019 , 12, 3532-3540	8.3	6
31	Towards optimal packing and diffusion of fullerene molecules in the Pc-PBBA covalent organic framework. <i>Molecular Simulation</i> , 2014 , 40, 58-70	2	6
30	Bypassing Solid-State Intermediates by Solvent Engineering the Crystallization Pathway in Hybrid Organic/Inorganic Perovskites. <i>Crystal Growth and Design</i> , 2020 , 20, 1162-1171	3.5	6
29	How well do implicit solvation models represent intermolecular binding energies in organic-inorganic solutions?. <i>Computational Materials Science</i> , 2019 , 170, 109138	3.2	5
28	Structural characterization of amorphous materials applied to low-k organosilicate materials. <i>Thin Solid Films</i> , 2014 , 562, 411-422	2.2	5
27	Simulation of graphene nanoribbon aggregation and its mediation by edge decoration. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 4766-76	3.4	5
26	Parameter-free correlation for a composition-based prediction of the dielectric constant of amorphous organosilicate materials. <i>Molecular Simulation</i> , 2012 , 38, 1221-1233	2	5
25	Chemical engineering in the electronics industry: progress towards the rational design of organic semiconductor heterojunctions. <i>Current Opinion in Chemical Engineering</i> , 2012 , 1, 117-122	5.4	5
24	A molecular dynamics study of the effect of pentacene polymorphs on C60 surface adsorption and diffusional properties and the tendency to form nanowires. <i>Molecular Simulation</i> , 2010 , 36, 590-603	2	5
23	Direct melt processing of pentacene at temperatures above 1000 °C by pulsed laser irradiation. <i>Applied Physics Letters</i> , 2008 , 93, 183306	3.4	5
22	Factors affecting tacticity and aggregation of P3HT polymers in P3HT:PCBM blends. <i>Molecular Simulation</i> , 2017 , 43, 743-755	2	4

21	The Role of Dimer Formation in the Nucleation of Superlattice Transformations and Its Impact on Disorder. <i>ACS Nano</i> , 2020 , 14, 11431-11441	16.7	4
20	Ab Initio Studies of the Diffusion of Intrinsic Defects and Silicon Dopants in Bulk InAs. <i>Langmuir</i> , 2017 , 33, 11484-11489	4	3
19	Preferred diffusional pathways of intrinsic defects and silicon dopants in an ordered phase of In _{0.5} Ga _{0.5} As: A first-principles study. <i>Acta Materialia</i> , 2017 , 140, 39-45	8.4	3
18	Effect of Laser Annealing on the Structure of Amorphous Porous SiCOH Materials. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 12616-12624	3.8	3
17	Organic Heterojunctions for Photovoltaic Applications: C ₆₀ Growth on Pentacene. <i>Materials Research Society Symposia Proceedings</i> , 2010 , 1263, 50601		3
16	A 3D model for simulating temperature and stress profiles during sub-millisecond laser spike annealing 2010 ,		3
15	Decomplexation as a rate limitation in the thiol-Michael addition of N-acrylamides. <i>Organic and Biomolecular Chemistry</i> , 2020 , 18, 6364-6377	3.9	3
14	SolventMolecule Interactions Govern Crystal-Habit Selection in Naphthalene Tetracarboxylic Diimides. <i>Chemistry of Materials</i> , 2019 , 31, 9691-9698	9.6	3
13	A new metric to control nucleation and grain size distribution in hybrid organicinorganic perovskites by tuning the dielectric constant of the antisolvent. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 3668-3676	13	3
12	Transferable Molecular Model of Woven Covalent Organic Framework Materials. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 48957-48968	9.5	2
11	Contorted Octabenzocircumbiphenyl Sorts Semiconducting Single-Walled Carbon Nanotubes with Structural Specificity. <i>Chemistry of Materials</i> , 2017 , 29, 595-604	9.6	1
10	Modeling the thermal poling of glasses using molecular dynamics. Part 2: Effects on elastic properties. <i>Journal of Non-Crystalline Solids</i> , 2017 , 468, 17-26	3.9	1
9	Simple Molecular Reactive Force Field for Metal-Organic Synthesis. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 825-38	6.4	1
8	A feasibility study of unconventional planar ligand spacers in chalcogenide nanocrystals. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 13781-93	3.6	1
7	Density functional theory studies of reaction mechanisms for titanium alkylamide incorporation onto functionalized aromatic self-assembled monolayers. <i>Journal of Materials Chemistry</i> , 2007 , 17, 3927		1
6	Evidence of Preformed Lewis AcidBase and Wheland-Type Complexes Acting as Dopants for p-Type Conjugated Polymers. <i>ACS Applied Polymer Materials</i> , 2022 , 4, 2065-2080	4.3	1
5	Fingerprinting the vibrational signatures of dopants and defects in a fully random alloy: An ab initio case study of Si, Se, and vacancies in In _{0.5} Ga _{0.5} As. <i>Journal of Applied Physics</i> , 2020 , 127, 205704	2.5	0
4	Development of a Suite of Computational Models for the Design of Ultralow-k SiCOH-based Materials. <i>Materials Research Society Symposia Proceedings</i> , 2012 , 1428, 45		

- 3 Dissolution and Growth Kinetics of Small Crystals in Liquids. *Materials Research Society Symposia Proceedings*, **1991**, 238, 279
- 2 Prediction of the Interface Response Functions for Amorphous and Crystalline Phases of Silicon and Germanium. *Materials Research Society Symposia Proceedings*, **2003**, 762, 1641
- 1 Resolving the mystery of the concentration-dependence of amphoteric dopant diffusion in III-V semiconductors. *Acta Materialia*, **2020**, 186, 555-563 8.4