Gabriele D'Avino

List of Publications by Year
in descending order

59 papers	2,498 citations	159585 30 h-index	197818 49 g-index
61 all docs	61 docs citations	61 times ranked	3235 citing authors

#	Article	IF	Citations
1	Highâ€Efficiency Ionâ€Exchange Doping of Conducting Polymers. Advanced Materials, 2022, 34, e2102988.	21.0	67
2	Dopingâ€Induced Dielectric Catastrophe Prompts Freeâ€Carrier Release in Organic Semiconductors. Advanced Materials, 2022, 34, e2105376.	21.0	9
3	Structural and Dynamic Disorder, Not Ionic Trapping, Controls Charge Transport in Highly Doped Conducting Polymers. Journal of the American Chemical Society, 2022, 144, 3005-3019.	13.7	45
4	Doping of semicrystalline conjugated polymers: dopants within alkyl chains do it better. Journal of Materials Chemistry C, 2022, 10, 13815-13825.	5.5	8
5	Electronâ€“Hole Separation in Perylene Diimide Based Self-Assembled Nanostructures: Microelectrostatics Analysis and Kinetic Monte Carlo Simulations. Journal of Physical Chemistry C, 2022, 126, 9762-9776.	3.1	3
6	Universal polarization energies for defects in monolayer, surface, and bulk hexagonal boron nitride: A finite-size fragments <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:m approach. Physical Review Materials, 2022, 6, .	2.4	9
7	Analysis of External and Internal Disorder to Understand Bandâ€Like Transport in nâ€Type Organic Semiconductors. Advanced Materials, 2021, 33, 2007870.	21.0	24
8	Bidimensional Hâ€Bond Network Promotes Structural Order and Electron Transport in BPyMPMs Molecular Semiconductor. Advanced Theory and Simulations, 2021, 4, 2000302.	2.8	4
9	Relaxor ferroelectricity in the polar M2P-TCNQ charge-transfer crystal at the neutral-ionic interface. Physical Review B, 2021, 103, .	3.2	3
10	Quantum Dynamics of Electronâ€“Hole Separation in Stacked Perylene Diimide-Based Self-Assembled Nanostructures. Journal of Physical Chemistry C, 2021, 125, 25030-25043.	3.1	6
11	Self-organization of complete organic monolayers via sequential post-deposition annealing. Progress in Organic Coatings, 2020, 138, 105408.	3.9	15
12	Fate of Low-Lying Charge-Transfer Excited States in a Donor:Acceptor Blend with a Large Energy Offset. Journal of Physical Chemistry Letters, 2020, 11, 10219-10226.	4.6	9
13	Charge transfer excitons in a donorâ€“acceptor amphidynamic crystal: the role of dipole orientational order. Materials Horizons, 2020, 7, 2951-2958.	12.2	8
14	Molecular Quadrupole Moments Promote Groundâ€State Charge Generation in Doped Organic Semiconductors. Advanced Functional Materials, 2020, 30, 2004600.	14.9	15
15	Orientation dependent molecular electrostatics drives efficient charge generation in homojunction organic solar cells. Nature Communications, 2020, 11, 4617.	12.8	60
16	Accurate Prediction of the S₁ Excitation Energy in Solvated Azobenzene Derivatives via Embedded Orbital-Tuned Bethe-Salpeter Calculations. Journal of Chemical Theory and Computation, 2020, 16, 2021-2027.	5.3	10
17	Electrostatic Interactions Shape Molecular Organization and Electronic Structure of Organic Semiconductor Blends. Chemistry of Materials, 2020, 32, 1261-1271.	6.7	24
18	Host dependence of the electron affinity of molecular dopants. Materials Horizons, 2019, 6, 107-114.	12.2	64

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19	Singlet exciton fission via an intermolecular charge transfer state in coevaporated pentacene-perfluoropentacene thin films. Journal of Chemical Physics, 2019, 151, 164706.	3.0	22
20	Chasing the â€œKillerâ€•Phonon Mode for the Rational Design of Lowâ€Disorder, Highâ€Mobility Molecular Semiconductors. Advanced Materials, 2019, 31, e1902407.	21.0	126
21	Multiple Charge Transfer States in Donorâ€“Acceptor Heterojunctions with Large Frontier Orbital Energy Offsets. Chemistry of Materials, 2019, 31, 6808-6817.	6.7	20
22	Electronic Structure, Electron-Phonon Coupling, and Charge Transport in Crystalline Rubrene Under Mechanical Strain. Journal of Physical Chemistry C, 2019, 123, 15897-15907.	3.1	22
23	Comprehensive modelling study of singlet exciton diffusion in donorâ€“acceptor dyads: when small changes in chemical structure matter. Physical Chemistry Chemical Physics, 2019, 21, 25023-25034.	2.8	14
24	Accurate description of charged excitations in molecular solids from embedded many-body perturbation theory. Physical Review B, 2018, 97, .	3.2	46
25	Rotator side chains trigger cooperative transition for shape and function memory effect in organic semiconductors. Nature Communications, 2018, 9, 278.	12.8	90
26	Pentacene Crystal Growth on Silica and Layer-Dependent Step-Edge Barrier from Atomistic Simulations. Journal of Physical Chemistry Letters, 2018, 9, 6900-6906.	4.6	25
27	Computational Design of Thermally Activated Delayed Fluorescence Materials: The Challenges Ahead. Journal of Physical Chemistry Letters, 2018, 9, 6149-6163.	4.6	121
28	Crystal step edges can trap electrons on the surfaces of n-type organic semiconductors. Nature Communications, 2018, 9, 2141.	12.8	55
29	Periodic potentials in hybrid van der Waals heterostructures formed by supramolecular lattices on graphene. Nature Communications, 2017, 8, 14767.	12.8	68
30	Energetic fluctuations in amorphous semiconducting polymers: Impact on charge-carrier mobility. Journal of Chemical Physics, 2017, 147, 134904.	3.0	21
31	Conflicting evidence for ferroelectricity. Nature, 2017, 547, E9-E10.	27.8	10
32	Towards first-principles prediction of valence instabilities in mixed stack charge-transfer crystals. Physical Review B, 2017, 95, .	3.2	16
33	Modeling the Neutral-Ionic Transition with Correlated Electrons Coupled to Soft Lattices and Molecules. Crystals, 2017, 7, 144.	2.2	14
34	Correlated electron-hole mechanism for molecular doping in organic semiconductors. Physical Review Materials, 2017, 1, .	2.4	42
35	Displacement of polarons by vibrational modes in doped conjugated polymers. Physical Review Materials, 2017, 1, .	2.4	27
36	Nature of the singlet and triplet excitations mediating thermally activated delayed fluorescence. Physical Review Materials, 2017, 1, .	2.4	102

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37	Dielectric properties of crystalline organic molecular films in the limit of zero overlap. Journal of Chemical Physics, 2016, 144, 034702.	3.0	11
38	Electrostatic phenomena in organic semiconductors: fundamentals and implications for photovoltaics. Journal of Physics Condensed Matter, 2016, 28, 433002.	1.8	131
39	Combining the Many-Body GW Formalism with Classical Polarizable Models: Insights on the Electronic Structure of Molecular Solids. Journal of Physical Chemistry Letters, 2016, 7, 2814-2820.	4.6	70
40	Charge Separation and Recombination at Polymerâ€“Fullerene Heterojunctions: Delocalization and Hybridization Effects. Journal of Physical Chemistry Letters, 2016, 7, 536-540.	4.6	93
41	Do charges delocalize over multiple molecules in fullerene derivatives?. Journal of Materials Chemistry C, 2016, 4, 3747-3756.	5.5	44
42	From Chiral Islands to Smectic Layers: A Computational Journey Across Sexithiophene Morphologies on C₆₀. Advanced Functional Materials, 2015, 25, 1985-1995.	14.9	32
43	Charge separation energetics at organic heterojunctions: on the role of structural and electrostatic disorder. Physical Chemistry Chemical Physics, 2014, 16, 20279-20290.	2.8	67
44	Electronic Polarization in Organic Crystals: A Comparative Study of Induced Dipoles and Intramolecular Charge Redistribution Schemes. Journal of Chemical Theory and Computation, 2014, 10, 4959-4971.	5.3	76
45	Are Hydrogen-Bonded Charge Transfer Crystals Room Temperature Ferroelectrics?. Physical Review Letters, 2014, 113, 237602.	7.8	35
46	Charge Dissociation at Interfaces between Discotic Liquid Crystals: The Surprising Role of Column Mismatch. Journal of the American Chemical Society, 2014, 136, 2911-2920.	13.7	55
47	Exploring the Energy Landscape of the Charge Transport Levels in Organic Semiconductors at the Molecular Scale. Accounts of Chemical Research, 2013, 46, 434-443.	15.6	64
48	Energetics of Electronâ€“Hole Separation at P3HT/PCBM Heterojunctions. Journal of Physical Chemistry C, 2013, 117, 12981-12990.	3.1	126
49	Bistability of Fc-PTM-Based Dyads: The Role of the Donor Strength. Chemistry of Materials, 2013, 25, 808-814.	6.7	45
50	Supramolecular Organization of Functional Organic Materials in the Bulk and at Organic/Organic Interfaces: A Modeling and Computer Simulation Approach. Topics in Current Chemistry, 2013, 352, 39-101.	4.0	18
51	Vibronic model for spin crossover complexes. Physical Review B, 2011, 84, .	3.2	41
52	Simulation of Vaporâ€Phase Deposition and Growth of a Pentacene Thin Film on C₆₀ (001). Advanced Materials, 2011, 23, 4532-4536.	21.0	90
53	Correlated electrons in soft lattices: Raman scattering evidence of the nonequilibrium dielectric divergence at the neutral-ionic phase transition. Physical Review B, 2011, 83, .	3.2	13
54	Essential State Models for Solvatochromism in Donorâ€'Acceptor Molecules: The Role of the Bridge. Journal of Physical Chemistry B, 2009, 113, 4718-4725.	2.6	42

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55	Cooperativity from electrostatic interactions: understanding bistability in molecular crystals. CrystEngComm, 2009, 11, 2040.	2.6	20
56	Bistability in Fc-PTM Crystals: The Role of Intermolecular Electrostatic Interactions. Journal of the American Chemical Society, 2008, 130, 12064-12072.	13.7	58
57	Anomalous Dispersion of Optical Phonons at the Neutral-Ionic Transition: Evidence from Diffuse X-Ray Scattering. Physical Review Letters, 2007, 99, 156407.	7.8	19
58	Multichromophores for Nonlinear Optics: Designing the Material Properties by Electrostatic Interactions. ChemPhysChem, 2007, 8, 2433-2444.	2.1	76
59	Aggregates of Quadrupolar Dyes:Â Giant Two-Photon Absorption from Biexciton States. Journal of Physical Chemistry B, 2006, 110, 25590-25592.	2.6	47