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	Electrostatic phenomena in organic semiconductors: fundamentals and implications for photovoltaics. Journal of Physics Condensed Matter, 2016, 28, 433002.	1.8	131
2	Energetics of Electronâ€“Hole Separation at P3HT/PCBM Heterojunctions. Journal of Physical Chemistry C, 2013, 117, 12981-12990.	3.1	126
3	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
4	Computational Design of Thermally Activated Delayed Fluorescence Materials: The Challenges Ahead. Journal of Physical Chemistry Letters, 2018, 9, 6149-6163.	4.6	121
5	Nature of the singlet and triplet excitations mediating thermally activated delayed fluorescence. Physical Review Materials, 2017, 1, .	2.4	102
6	Charge Separation and Recombination at Polymerâ€“Fullerene Heterojunctions: Delocalization and Hybridization Effects. Journal of Physical Chemistry Letters, 2016, 7, 536-540.	4.6	93
7	Simulation of Vaporâ€Phase Deposition and Growth of a Pentacene Thin Film on C₆₀ (001). Advanced Materials, 2011, 23, 4532-4536.	21.0	90
8	Rotator side chains trigger cooperative transition for shape and function memory effect in organic semiconductors. Nature Communications, 2018, 9, 278.	12.8	90
9	Multichromophores for Nonlinear Optics: Designing the Material Properties by Electrostatic Interactions. ChemPhysChem, 2007, 8, 2433-2444.	2.1	76
10	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
11	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
12	Periodic potentials in hybrid van der Waals heterostructures formed by supramolecular lattices on graphene. Nature Communications, 2017, 8, 14767.	12.8	68
13	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
14	Highâ€Efficiency Ionâ€Exchange Doping of Conducting Polymers. Advanced Materials, 2022, 34, e2102988.	21.0	67
15	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
16	Host dependence of the electron affinity of molecular dopants. Materials Horizons, 2019, 6, 107-114.	12.2	64
17	Orientation dependent molecular electrostatics drives efficient charge generation in homojunction organic solar cells. Nature Communications, 2020, 11, 4617.	12.8	60
18	Bistability in Fc-PTM Crystals: The Role of Intermolecular Electrostatic Interactions. Journal of the American Chemical Society, 2008, 130, 12064-12072.	13.7	58

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19	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
20	Crystal step edges can trap electrons on the surfaces of n-type organic semiconductors. Nature Communications, 2018, 9, 2141.	12.8	55
21	Aggregates of Quadrupolar Dyes:Â Giant Two-Photon Absorption from Biexciton States. Journal of Physical Chemistry B, 2006, 110, 25590-25592.	2.6	47
22	Accurate description of charged excitations in molecular solids from embedded many-body perturbation theory. Physical Review B, 2018, 97, .	3.2	46
23	Bistability of Fc-PTM-Based Dyads: The Role of the Donor Strength. Chemistry of Materials, 2013, 25, 808-814.	6.7	45
24	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
25	Do charges delocalize over multiple molecules in fullerene derivatives?. Journal of Materials Chemistry C, 2016, 4, 3747-3756.	5.5	44
26	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
27	Correlated electron-hole mechanism for molecular doping in organic semiconductors. Physical Review Materials, 2017, 1, .	2.4	42
28	Vibronic model for spin crossover complexes. Physical Review B, 2011, 84, .	3.2	41
29	Are Hydrogen-Bonded Charge Transfer Crystals Room Temperature Ferroelectrics?. Physical Review Letters, 2014, 113, 237602.	7.8	35
30	From Chiral Islands to Smectic Layers: A Computational Journey Across Sexithiophene Morphologies on C₆₀. Advanced Functional Materials, 2015, 25, 1985-1995.	14.9	32
31	Displacement of polarons by vibrational modes in doped conjugated polymers. Physical Review Materials, 2017, 1, .	2.4	27
32	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
33	Electrostatic Interactions Shape Molecular Organization and Electronic Structure of Organic Semiconductor Blends. Chemistry of Materials, 2020, 32, 1261-1271.	6.7	24
34	Analysis of External and Internal Disorder to Understand Bandâ€Like Transport in nâ€Type Organic Semiconductors. Advanced Materials, 2021, 33, 2007870.	21.0	24
35	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
36	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

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37	Energetic fluctuations in amorphous semiconducting polymers: Impact on charge-carrier mobility. Journal of Chemical Physics, 2017, 147, 134904.	3.0	21
38	Cooperativity from electrostatic interactions: understanding bistability in molecular crystals. CrystEngComm, 2009, 11, 2040.	2.6	20
39	Multiple Charge Transfer States in Donorâ€“Acceptor Heterojunctions with Large Frontier Orbital Energy Offsets. Chemistry of Materials, 2019, 31, 6808-6817.	6.7	20
40	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
41	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
42	Towards first-principles prediction of valence instabilities in mixed stack charge-transfer crystals. Physical Review B, 2017, 95, .	3.2	16
43	Self-organization of complete organic monolayers via sequential post-deposition annealing. Progress in Organic Coatings, 2020, 138, 105408.	3.9	15
44	Molecular Quadrupole Moments Promote Groundâ€State Charge Generation in Doped Organic Semiconductors. Advanced Functional Materials, 2020, 30, 2004600.	14.9	15
45	Modeling the Neutral-Ionic Transition with Correlated Electrons Coupled to Soft Lattices and Molecules. Crystals, 2017, 7, 144.	2.2	14
46	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
47	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
48	Dielectric properties of crystalline organic molecular films in the limit of zero overlap. Journal of Chemical Physics, 2016, 144, 034702.	3.0	11
49	Conflicting evidence for ferroelectricity. Nature, 2017, 547, E9-E10.	27.8	10
50	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
51	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
52	Dopingâ€Induced Dielectric Catastrophe Prompts Freeâ€Carrier Release in Organic Semiconductors. Advanced Materials, 2022, 34, e2105376.	21.0	9
53	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 approach. Physical Review Materials, 2022, 6, .	2.4	9
54	Charge transfer excitons in a donorâ€“acceptor amphidynamic crystal: the role of dipole orientational order. Materials Horizons, 2020, 7, 2951-2958.	12.2	8

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55	Doping of semicrystalline conjugated polymers: dopants within alkyl chains do it better. Journal of Materials Chemistry C, 2022, 10, 13815-13825.	5.5	8
56	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
57	Bidimensional Hâ€Bond Network Promotes Structural Order and Electron Transport in BPyMPMs Molecular Semiconductor. Advanced Theory and Simulations, 2021, 4, 2000302.	2.8	4
58	Relaxor ferroelectricity in the polar M2P-TCNQ charge-transfer crystal at the neutral-ionic interface. Physical Review B, 2021, 103, .	3.2	3
59	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