

# Angelo Gavezzotti

## List of Publications by Year in descending order

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52  
papers

3,750  
citations

236912  
25  
h-index

233409  
45  
g-index

52  
all docs

52  
docs citations

52  
times ranked

3419  
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular dynamics simulation of organic materials: structure, potentials and the MiCMoS computer platform. CrystEngComm, 2022, 24, 922-930.	2.6	8
2	The crystalline state of rubrene materials: intermolecular recognition, isomorphism, polymorphism, and periodic bond-chain analysis of morphologies. New Journal of Chemistry, 2022, 46, 7626-7637.	2.8	4
3	Dynamic simulation of orientational disorder in organic crystals: methyl groups, trifluoromethyl groups and whole molecules. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2022, 78, 333-343.	1.1	4
4	Kinetic-Bias Model for the Dynamic Simulation of Molecular Aggregation. The Liquid, Solute, Solvated-Nanodrop, and Solvated-Nanocrystal States of Benzoic Acid. Crystal Growth and Design, 2022, 22, 1857-1866.	3.0	5
5	Collective Variables for the Simulation of Crystallization of Organic Compounds: Some Case Studies. Israel Journal of Chemistry, 2021, 61, 498.	2.3	1
6	Crystal structure prediction from molecular structure: Highlights and shadows. Theoretical and Computational Chemistry, 2021, 20, 115-142.	0.4	1
7	The intermolecular chemical bond: Physical facts and geometric fiction. Theoretical and Computational Chemistry, 2021, 20, 25-52.	0.4	0
8	Multi-molecular asymmetric units and cocrystals: Symmetry violation. Theoretical and Computational Chemistry, 2021, , 169-199.	0.4	0
9	The organic crystal potential: History, development, and today's cost/performance ratios. Theoretical and Computational Chemistry, 2021, 20, 85-113.	0.4	0
10	X-ray analysis of crystals and the Cambridge structural database: Use and better uses. Theoretical and Computational Chemistry, 2021, , 53-83.	0.4	0
11	Organic crystal nucleation and growth: Little knowledge, much mystery. Theoretical and Computational Chemistry, 2021, 20, 201-229.	0.4	1
12	The dynamic simulation of aggregate chemical systems: Use and misuse of long lists of numbers. Theoretical and Computational Chemistry, 2021, 20, 231-265.	0.4	0
13	Molecular Dynamics Simulation of Molecular Crystals under Anisotropic Compression: Bulk and Directional Effects in Anthracene and Paracetamol. Crystal Growth and Design, 2020, 20, 7421-7428.	3.0	6
14	Mining the Cambridge Database for theoretical chemistry. Mi-LJC: a new set of Lennard-Jones–Coulomb atom–atom potentials for the computer simulation of organic condensed matter. CrystEngComm, 2020, 22, 7350-7360.	2.6	17
15	Sublimation Enthalpies of Organic Compounds: A Very Large Database with a Match to Crystal Structure Determinations and a Comparison with Lattice Energies. Crystal Growth and Design, 2019, 19, 6566-6576.	3.0	23
16	Dynamic simulation of liquid molecular nanoclusters: structure, stability and quantification of internal (pseudo)symmetries. New Journal of Chemistry, 2019, 43, 2077-2084.	2.8	11
17	Molecular dynamics simulation of organic crystals: introducing the CLP-dyncry environment. Journal of Applied Crystallography, 2019, 52, 1253-1263.	4.5	17
18	Pillars of crystal engineering: crystal energies and symmetry operators. CrystEngComm, 2018, 20, 2511-2518.	2.6	8

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19	The TACO Puzzle: A Phase-Transition Mystery Revisited. <i>Crystal Growth and Design</i> , 2018, 18, 7219-7227.	3.0	5
20	Two-component organic crystals without hydrogen bonding: structure and intermolecular interactions in bimolecular stacking. <i>CrystEngComm</i> , 2017, 19, 2413-2423.	2.6	30
21	A quantitative measure of halogen bond activation in cocrystallization. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 18383-18388.	2.8	14
22	Building Blocks of Crystal Engineering: A Large-Database Study of the Intermolecular Approach between C-H Donor Groups and O, N, Cl, or F Acceptors in Organic Crystals. <i>Crystal Growth and Design</i> , 2016, 16, 2952-2962.	3.0	57
23	Facts and Factors in the Formation and Stability of Binary Crystals. <i>Crystal Growth and Design</i> , 2016, 16, 6095-6104.	3.0	43
24	Comparing the strength of covalent bonds, intermolecular hydrogen bonds and other intermolecular interactions for organic molecules: X-ray diffraction data and quantum chemical calculations. <i>New Journal of Chemistry</i> , 2016, 40, 6848-6853.	2.8	41
25	Theoretical Study of Chiral Carboxylic Acids. Structural and Energetic Aspects of Crystalline and Liquid States. <i>Crystal Growth and Design</i> , 2015, 15, 3792-3803.	3.0	64
26	Are Racemic Crystals Favored over Homochiral Crystals by Higher Stability or by Kinetics? Insights from Comparative Studies of Crystalline Stereoisomers. <i>Journal of Organic Chemistry</i> , 2014, 79, 4809-4816.	3.2	41
27	Molecular Level Insights on the Liquid-Solid Transition of Large Organics by Biased Monte Carlo Simulations. <i>Crystal Growth and Design</i> , 2013, 13, 3801-3815.	3.0	10
28	Equilibrium structure and dynamics of organic crystals by Monte Carlo simulation: critical assessment of force fields and comparison with static packing analysis. <i>New Journal of Chemistry</i> , 2013, 37, 2110.	2.8	25
29	The "conceptual chymist's" intermolecular doubts and paradoxes. <i>CrystEngComm</i> , 2013, 15, 4027.	2.6	89
30	Can a computer crystallize a liquid? Molecular simulation of continuous trajectories from liquid to crystalline n-hexane. <i>CrystEngComm</i> , 2011, 13, 3573.	2.6	15
31	Intermolecular Interaction Energies in Molecular Crystals: Comparison and Agreement of Localized Møller-Plesset 2, Dispersion-Corrected Density Functional, and Classical Empirical Two-Body Calculations. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11179-11186.	2.5	169
32	Efficient computer modeling of organic materials. The atom-atom, Coulomb-London-Pauli (AA-CLP) model for intermolecular electrostatic-polarization, dispersion and repulsion energies. <i>New Journal of Chemistry</i> , 2011, 35, 1360.	2.8	322
33	How molecules stick together in organic crystals: weak intermolecular interactions. <i>Chemical Society Reviews</i> , 2009, 38, 2622.	38.1	277
34	Competition between hydrogen bonding and arene-perfluoroarene stacking. X-Ray diffraction and molecular simulation on 5,6,7,8-tetrafluoro-2-naphthoic acid and 5,6,7,8-tetrafluoro-2-naphthamide crystals. <i>CrystEngComm</i> , 2009, 11, 1122.	2.6	22
35	Hydrogen bond strength and bond geometry in cyclic dimers of crystalline carboxylic acids. <i>Acta Crystallographica Section B: Structural Science</i> , 2008, 64, 401-403.	1.8	31
36	Polymorphic Perversity: Crystal Structures with Many Symmetry-Independent Molecules in the Unit Cell. <i>Crystal Growth and Design</i> , 2008, 8, 2011-2018.	3.0	96

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37	Non-conventional bonding between organic molecules. The 'halogen bond' in crystalline systems. <i>Molecular Physics</i> , 2008, 106, 1473-1485.	1.7	216
38	Computer Simulations and Analysis of Structural and Energetic Features of Some Crystalline Energetic Materials. <i>Journal of Physical Chemistry B</i> , 2007, 111, 3430-3437.	2.6	67
39	Synthesis, X-ray Diffraction and Computational Study of the Crystal Packing of Polycyclic Hydrocarbons Featuring Aromatic and Perfluoroaromatic Rings Condensed in the Same Molecule: 1,2,3,4-Tetrafluoronaphthalene, -anthracene and -phenanthrene. <i>Chemistry - A European Journal</i> , 2007, 13, 7177-7184.	3.3	74
40	Molecular Recognition in Organic Crystals: Directed Intermolecular Bonds or Nonlocalized Bonding?. <i>Angewandte Chemie - International Edition</i> , 2005, 44, 1766-1787.	13.8	403
41	Toward a Quantitative Description of Crystal Packing in Terms of Molecular Pairs: Application to the Hexamorphic Crystal System, 5-Methyl-2-[(2-nitrophenyl)amino]-3-thiophenecarbonitrile. <i>Crystal Growth and Design</i> , 2005, 5, 2180-2189.	3.0	91
42	Cocrystallization with Acetylene. The 1:1 Complex with Benzene: Crystal Growth, X-Ray Diffraction and Molecular Simulations. <i>Helvetica Chimica Acta</i> , 2003, 86, 1085-1100.	1.6	59
43	Towards a realistic model for the quantitative evaluation of intermolecular potentials and for the rationalization of organic crystal structures. Part I. Philosophy Electronic Supplementary Information (ESI) is available: the GAUSSIAN input files, the Pixel-SCDS input and output files have been deposited. See <a href="http://www.rsc.org/suppdata/ce/b3/b311831b/">http://www.rsc.org/suppdata/ce/b3/b311831b/</a> . <i>CrystEngComm</i> , 2003, 5, 429.	2.6	90
44	X-ray Diffraction and Molecular Simulation Study of the Crystalline and Liquid States of Succinic Anhydride. <i>Chemistry - A European Journal</i> , 2002, 8, 1710-1718.	3.3	17
45	A test of crystal structure prediction of small organic molecules. <i>Acta Crystallographica Section B: Structural Science</i> , 2000, 56, 697-714.	1.8	376
46	Attractions and Repulsions in Molecular Crystals: What Can Be Learned from the Crystal Structures of Condensed Ring Aromatic Hydrocarbons?. <i>Accounts of Chemical Research</i> , 1999, 32, 677-684.	15.6	186
47	Orthorhombic and Monoclinic 2,3,7,8-Tetramethoxythianthrene: Small Structural Difference Large Lattice Change. <i>Angewandte Chemie International Edition in English</i> , 1995, 34, 76-78.	4.4	12
48	Molecular symmetry, melting temperatures and melting enthalpies of substituted benzenes and naphthalenes. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1995, , 1399.	0.9	53
49	Geometry of the Intermolecular X-H...Y (X, Y = N, O) Hydrogen Bond and the Calibration of Empirical Hydrogen-Bond Potentials. <i>The Journal of Physical Chemistry</i> , 1994, 98, 4831-4837.	2.9	390
50	Empirical intermolecular potentials for organic crystals: the '6-exp' approximation revisited. <i>Acta Crystallographica Section B: Structural Science</i> , 1993, 49, 868-880.	1.8	203
51	Molecular rearrangements in organic crystals. I. Potential energy calculations for some cases of reorientational disorder. <i>The Acta Crystallographica Section A, Crystal Physics, Diffraction and General Crystallography</i> , 1975, 31, 645-654.	0.6	56
52	Crystallography without Crystals: A Structural Study of Fakein. <i>Helvetica Chimica Acta</i> , 0, , .	1.6	0