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 Recognition in Organic Crystals: Directed Intermolecular Bonds or Nonlocalized Bonding?. Angewandte Chemie - International Edition, 2005, 44, 1766-1787.	13.8	403
2	Geometry of the Intermolecular X-H.cntdot..cntdot..cntdot.Y (X, Y = N, O) Hydrogen Bond and the Calibration of Empirical Hydrogen-Bond Potentials. The Journal of Physical Chemistry, 1994, 98, 4831-4837.	2.9	390
3	A test of crystal structure prediction of small organic molecules. Acta Crystallographica Section B: Structural Science, 2000, 56, 697-714.	1.8	376
4	Efficient computer modeling of organic materials. The atomâ€“atom, Coulombâ€“Londonâ€“Pauli (AA-CLP) model for intermolecular electrostatic-polarization, dispersion and repulsion energies. New Journal of Chemistry, 2011, 35, 1360.	2.8	322
5	How molecules stick together in organic crystals: weak intermolecular interactions. Chemical Society Reviews, 2009, 38, 2622.	38.1	277
6	Non-conventional bonding between organic molecules. The 'halogen bond' in crystalline systems. Molecular Physics, 2008, 106, 1473-1485.	1.7	216
7	Empirical intermolecular potentials for organic crystals: the `6-exp' approximation revisited. Acta Crystallographica Section B: Structural Science, 1993, 49, 868-880.	1.8	203
8	Attractions and Repulsions in Molecular Crystals:Â What Can Be Learned from the Crystal Structures of Condensed Ring Aromatic Hydrocarbons?. Accounts of Chemical Research, 1999, 32, 677-684.	15.6	186
9	Intermolecular Interaction Energies in Molecular Crystals: Comparison and Agreement of Localized MÃ¸llerâ€“Plesset 2, Dispersion-Corrected Density Functional, and Classical Empirical Two-Body Calculations. Journal of Physical Chemistry A, 2011, 115, 11179-11186.	2.5	169
10	Polymorphic Perversity: Crystal Structures with Many Symmetry-Independent Molecules in the Unit Cell. Crystal Growth and Design, 2008, 8, 2011-2018.	3.0	96
11	Toward a Quantitative Description of Crystal Packing in Terms of Molecular Pairs:â€‰ Application to the Hexamorphic Crystal System, 5-Methyl-2-[(2-nitrophenyl)amino]-3-thiophenecarbonitrileâ€. Crystal Growth and Design, 2005, 5, 2180-2189.	3.0	91
12	Towards a realistic model for the quantitative evaluation of intermolecular potentials and for the rationalization of organic crystal structures. Part I. PhilosophyElectronic Supplementary Information (ESI) is available: the GAUSSIAN input files, the Pixel-SCDS input and output files have been deposited. See http://www.rsc.org/suppdata/ce/b3/b311831b/. CrystEngComm, 2003, 5, 429.	2.6	90
13	The â€œsceptical chymistâ€• intermolecular doubts and paradoxes. CrystEngComm, 2013, 15, 4027.	2.6	89
14	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. Chemistry - A European Journal, 2007, 13, 7177-7184.	3.3	74
15	Computer Simulations and Analysis of Structural and Energetic Features of Some Crystalline Energetic Materials. Journal of Physical Chemistry B, 2007, 111, 3430-3437.	2.6	67
16	Theoretical Study of Chiral Carboxylic Acids. Structural and Energetic Aspects of Crystalline and Liquid States. Crystal Growth and Design, 2015, 15, 3792-3803.	3.0	64
17	Cocrystallization with Acetylene. The 1â€‰:â€‰1 Complex with Benzene: Crystal Growth, X-Ray Diffraction and Molecular Simulations. Helvetica Chimica Acta, 2003, 86, 1085-1100.	1.6	59
18	Building Blocks of Crystal Engineering: A Large-Database Study of the Intermolecular Approach between Câ€“H Donor Groups and O, N, Cl, or F Acceptors in Organic Crystals. Crystal Growth and Design, 2016, 16, 2952-2962.	3.0	57

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19	Molecular rearrangements in organic crystals. I. Potential energy calculations for some cases of reorientational disorder. The Acta Crystallographica Section A, Crystal Physics, Diffractionoretical and General Crystallography, 1975, 31, 645-654.	0.6	56
20	Molecular symmetry, melting temperatures and melting enthalpies of substituted benzenes and naphthalenes. Journal of the Chemical Society Perkin Transactions II, 1995, , 1399.	0.9	53
21	Facts and Factors in the Formation and Stability of Binary Crystals. Crystal Growth and Design, 2016, 16, 6095-6104.	3.0	43
22	Are Racemic Crystals Favored over Homochiral Crystals by Higher Stability or by Kinetics? Insights from Comparative Studies of Crystalline Stereoisomers. Journal of Organic Chemistry, 2014, 79, 4809-4816.	3.2	41
23	Comparing the strength of covalent bonds, intermolecular hydrogen bonds and other intermolecular interactions for organic molecules: X-ray diffraction data and quantum chemical calculations. New Journal of Chemistry, 2016, 40, 6848-6853.	2.8	41
24	Hydrogen bond strength and bond geometry in cyclic dimers of crystalline carboxylic acids. Acta Crystallographica Section B: Structural Science, 2008, 64, 401-403.	1.8	31
25	Two-component organic crystals without hydrogen bonding: structure and intermolecular interactions in bimolecular stacking. CrystEngComm, 2017, 19, 2413-2423.	2.6	30
26	Equilibrium structure and dynamics of organic crystals by Monte Carlo simulation: critical assessment of force fields and comparison with static packing analysis. New Journal of Chemistry, 2013, 37, 2110.	2.8	25
27	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
28	Competition between hydrogen bonding and areneâ€“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. CrystEngComm, 2009, 11, 1122.	2.6	22
29	X-ray Diffraction and Molecular Simulation Study of the Crystalline and Liquid States of Succinic Anhydride. Chemistry - A European Journal, 2002, 8, 1710-1718.	3.3	17
30	Molecular dynamics simulation of organic crystals: introducing the CLP-dyncry environment. Journal of Applied Crystallography, 2019, 52, 1253-1263.	4.5	17
31	Mining the Cambridge Database for theoretical chemistry. Mi-LJC: a new set of Lennard-Jonesâ€“Coulomb atomâ€“atom potentials for the computer simulation of organic condensed matter. CrystEngComm, 2020, 22, 7350-7360.	2.6	17
32	Can a computer crystallize a liquid? Molecular simulation of continuous trajectories from liquid to crystalline n-hexane. CrystEngComm, 2011, 13, 3573.	2.6	15
33	A quantitative measure of halogen bond activation in cocrystallization. Physical Chemistry Chemical Physics, 2017, 19, 18383-18388.	2.8	14
34	Orthorhombic and Monoclinic 2,3,7,8-Tetramethoxythianthrene: Small Structural Differenceâ€“Large Lattice Change. Angewandte Chemie International Edition in English, 1995, 34, 76-78.	4.4	12
35	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
36	Molecular Level Insights on the Liquidâ€“Solid Transition of Large Organics by Biased Monte Carlo Simulations. Crystal Growth and Design, 2013, 13, 3801-3815.	3.0	10

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37	Pillars of crystal engineering: crystal energies and symmetry operators. CrystEngComm, 2018, 20, 2511-2518.	2.6	8
38	Molecular dynamics simulation of organic materials: structure, potentials and the MiCMoS computer platform. CrystEngComm, 2022, 24, 922-930.	2.6	8
39	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
40	The TACO Puzzle: A Phase-Transition Mystery Revisited. Crystal Growth and Design, 2018, 18, 7219-7227.	3.0	5
41	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
42	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
43	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
44	Collective Variables for the Simulation of Crystallization of Organic Compounds: Some Case Studies. Israel Journal of Chemistry, 2021, 61, 498.	2.3	1
45	Crystal structure prediction from molecular structure: Highlights and shadows. Theoretical and Computational Chemistry, 2021, 20, 115-142.	0.4	1
46	Organic crystal nucleation and growth: Little knowledge, much mystery. Theoretical and Computational Chemistry, 2021, 20, 201-229.	0.4	1
47	The intermolecular chemical bond: Physical facts and geometric fiction. Theoretical and Computational Chemistry, 2021, 20, 25-52.	0.4	0
48	Multi-molecular asymmetric units and cocrystals: Symmetry violation. Theoretical and Computational Chemistry, 2021, , 169-199.	0.4	0
49	The organic crystal potential: History, development, and today's cost/performance ratios. Theoretical and Computational Chemistry, 2021, 20, 85-113.	0.4	0
50	X-ray analysis of crystals and the Cambridge structural database: Use and better uses. Theoretical and Computational Chemistry, 2021, , 53-83.	0.4	0
51	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
52	Crystallography without Crystals: A Structural Study of Fakein. Helvetica Chimica Acta, 0, , .	1.6	0