# Angelo Gavezzotti

List of Publications by Year
in descending order

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| 52 | 3,750 | 270111 | 263392 |
|---|---|---|---|
| papers | citations | 25 h-index | 45 g-index |

| 52 | 52 | 52 | 3789 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Molecular dynamics simulation of organic materials: structure, potentials and the MiCMoS computer platform. CrystEngComm, 2022, 24, 922-930. | 1.3 | 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. | 1.4 | 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. | 0.5 | 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. | 1.4 | 5 |
| 5 | Collective Variables for the Simulation of Crystallization of Organic Compounds: Some Case Studies. Israel Journal of Chemistry, 2021, 61, 498. | 1.0 | 1 |
| 6 | Crystal structure prediction from molecular structure: Highlights and shadows. Theoretical and Computational Chemistry, 2021, 20, 115-142. | 0.2 | 1 |
| 7 | The intermolecular chemical bond: Physical facts and geometric fiction. Theoretical and Computational Chemistry, 2021, 20, 25-52. | 0.2 | 0 |
| 8 | Multi-molecular asymmetric units and cocrystals: Symmetry violation. Theoretical and Computational Chemistry, 2021, , 169-199. | 0.2 | 0 |
| 9 | The organic crystal potential: History, development, and today's cost/performance ratios. Theoretical and Computational Chemistry, 2021, 20, 85-113. | 0.2 | 0 |
| 10 | X-ray analysis of crystals and the Cambridge structural database: Use and better uses. Theoretical and Computational Chemistry, 2021, , 53-83. | 0.2 | 0 |
| 11 | Organic crystal nucleation and growth: Little knowledge, much mystery. Theoretical and Computational Chemistry, 2021, 20, 201-229. | 0.2 | 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. | 0.2 | 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. | 1.4 | 6 |
| 14 | 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. | 1.3 | 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. | 1.4 | 23 |
| 16 | Dynamic simulation of liquid molecular nanoclusters: structure, stability and quantification of internal (pseudo)symmetries. New Journal of Chemistry, 2019, 43, 2077-2084. | 1.4 | 11 |
| 17 | Molecular dynamics simulation of organic crystals: introducing the CLP-dyncry environment. Journal of Applied Crystallography, 2019, 52, 1253-1263. | 1.9 | 17 |
| 18 | Pillars of crystal engineering: crystal energies and symmetry operators. CrystEngComm, 2018, 20, 2511-2518. | 1.3 | 8 |

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|---|---|---|---|
| 19 | The TACO Puzzle: A Phase-Transition Mystery Revisited. Crystal Growth and Design, 2018, 18, 7219-7227. | 1.4 | 5 |
| 20 | Two-component organic crystals without hydrogen bonding: structure and intermolecular interactions in bimolecular stacking. CrystEngComm, 2017, 19, 2413-2423. | 1.3 | 30 |
| 21 | A quantitative measure of halogen bond activation in cocrystallization. Physical Chemistry Chemical Physics, 2017, 19, 18383-18388. | 1.3 | 14 |
| 22 | 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. | 1.4 | 57 |
| 23 | Facts and Factors in the Formation and Stability of Binary Crystals. Crystal Growth and Design, 2016, 16, 6095-6104. | 1.4 | 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. New Journal of Chemistry, 2016, 40, 6848-6853. | 1.4 | 41 |
| 25 | Theoretical Study of Chiral Carboxylic Acids. Structural and Energetic Aspects of Crystalline and Liquid States. Crystal Growth and Design, 2015, 15, 3792-3803. | 1.4 | 64 |
| 26 | 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. | 1.7 | 41 |
| 27 | Molecular Level Insights on the Liquidâ€“Solid Transition of Large Organics by Biased Monte Carlo Simulations. Crystal Growth and Design, 2013, 13, 3801-3815. | 1.4 | 10 |
| 28 | 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. | 1.4 | 25 |
| 29 | The â€œsceptical chymistâ€: intermolecular doubts and paradoxes. CrystEngComm, 2013, 15, 4027. | 1.3 | 89 |
| 30 | Can a computer crystallize a liquid? Molecular simulation of continuous trajectories from liquid to crystalline n-hexane. CrystEngComm, 2011, 13, 3573. | 1.3 | 15 |
| 31 | 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. | 1.1 | 169 |
| 32 | 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. | 1.4 | 322 |
| 33 | How molecules stick together in organic crystals: weak intermolecular interactions. Chemical Society Reviews, 2009, 38, 2622. | 18.7 | 277 |
| 34 | 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. | 1.3 | 22 |
| 35 | 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 |
| 36 | Polymorphic Perversity: Crystal Structures with Many Symmetry-Independent Molecules in the Unit Cell. Crystal Growth and Design, 2008, 8, 2011-2018. | 1.4 | 96 |

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|---|---|---|---|
| 37 | Non-conventional bonding between organic molecules. The 'halogen bond' in crystalline systems. Molecular Physics, 2008, 106, 1473-1485. | 0.8 | 216 |
| 38 | Computer Simulations and Analysis of Structural and Energetic Features of Some Crystalline Energetic Materials. Journal of Physical Chemistry B, 2007, 111, 3430-3437. | 1.2 | 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. Chemistry - A European Journal, 2007, 13, 7177-7184. | 1.7 | 74 |
| 40 | Molecular Recognition in Organic Crystals: Directed Intermolecular Bonds or Nonlocalized Bonding?. Angewandte Chemie - International Edition, 2005, 44, 1766-1787. | 7.2 | 403 |
| 41 | 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. | 1.4 | 91 |
| 42 | 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. | 1.0 | 59 |
| 43 | 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. | 1.3 | 90 |
| 44 | X-ray Diffraction and Molecular Simulation Study of the Crystalline and Liquid States of Succinic Anhydride. Chemistry - A European Journal, 2002, 8, 1710-1718. | 1.7 | 17 |
| 45 | A test of crystal structure prediction of small organic molecules. Acta Crystallographica Section B: Structural Science, 2000, 56, 697-714. | 1.8 | 376 |
| 46 | 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. | 7.6 | 186 |
| 47 | 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 |
| 48 | 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 |
| 49 | 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 |
| 50 | Empirical intermolecular potentials for organic crystals: the `6-exp' approximation revisited. Acta Crystallographica Section B: Structural Science, 1993, 49, 868-880. | 1.8 | 203 |
| 51 | 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 |
| 52 | Crystallography without Crystals: A Structural Study of Fakein. Helvetica Chimica Acta, 0, , . | 1.0 | 0 |