

Angelo Gavezzotti List of publications

Articles

Entries referring to full papers in properly refereed Journals are numbered consecutively in order of appearance. Entries without a sequence number refer to Conference proceedings, miscellaneous papers, or articles in Journals and books without refereeing

1) Casalone, G.; Gavezzotti, A.; Mariani, C.; Mugnoli, A.; Simonetta, M.
The Crystal Structure of 1,1-di-*p*-tolylethylene
Acta Crystallogr. **1970**, B26, 1-8.

2) Casalone, G.; Gavezzotti, A.; Mugnoli, A.; Simonetta, M.
Kristallstruktur von 1,6:8,13-propanediyliden[14]annulene
*Angew.Chem.***1970**, 82, 516-517; *Angew.Chem.Int.Ed.Engl.* **1970**, 9, 519-520.

Casalone, G.; Gavezzotti, A.
Conformational Analysis of the 1,1-di-*p*-Tolylethylene Molecule
Rendiconti Istituto Lombardo, Acc.Sc.Lett., Cl.Sci. (A), **1971**, 105, 824-833.

3) Gavezzotti, A.; Mugnoli, A.; Raimondi, M.; Simonetta, M.
Crystal and molecular structure of 1,6:8,13-propanediylidene[14]annulene
J.Chem.Soc.Perkin II **1972**, 425-431.

4) Gavezzotti, A.; Gramaccioli, C.M.
Symmetry Considerations with respect to Space-Group Extinctions
and Weights in Intensity Statistics
Acta Crystallogr. **1973**, A29, 213-214.

Bianchi, R.; Destro, R.; Gavezzotti, A.
A set of programs for the application of direct methods in Crystallography
*Atti Accad. Naz. Lincei, Rendic. Cl. Sci. Fis. Mat. Natur.***1972**, Ser.VIII, 52, 114-119.

5) Beringhelli, T.; Gavezzotti, A.; Simonetta, M.
Semiempirical calculations on the thermal cis-trans isomerization of 2-butene,2-pentene,
methylstyrene and stilbene
*J. Mol. Struct.***1972**, 12, 333-342.

Beringhelli, T.; Gavezzotti, A.
Calcolo delle stabilita' relative dei cationi omoallilici ed omobenzilici
Rendiconti Istituto Lombardo, Acc.Sc.Lett., Cl.Sci. (A), **1973**, 107, 148-154.

6) Casalone, G.; Gavezzotti, A.; Simonetta, M.
Molecular Structure of *p*-Nitrobiphenyl. A Comparison of the Results of X-Ray Crystal
Analysis with Semi-empirical Calculations of Conformation
J.Chem.Soc.Perkin II **1973**,342-345

- 7) Beltrame, P.; Gavezzotti, A.; Simonetta, M.
Reaction of Haloacetylenes with Sulphur Nucleophiles studied by Extended Hückel
Molecular Orbital Theory
J.Chem.Soc.Perkin II **1974**, 502-507.
- 8) Gavezzotti, A.; Simonetta, M.
Orbital symmetry rules and steric hindrance in the thermal 1,3 sigmatropic rearrangement of
bicyclo[3.2.0]heptenes to norbornenes. Extended Hückel Calculations
Tetrahedron **1975**, 31,1611-1617.
- 9) Gavezzotti, A.; Simonetta, M.
Molecular Rearrangements in Organic Crystals. I. Potential Energy Calculations for Some
Cases of Reorientational Disorder
Acta Crystallogr. **1975**, A31, 645-654.
- 10) Gavezzotti, A.; Simonetta, M.
Substituents effects in optical and geometrical isomerization of cyclopropanes
Tetrahedron Lett. **1975**, 4155-4158.
- Gavezzotti, A.; Simonetta, M.
Conformational analysis of some overcrowded olefins
Atti Accad. Naz. Lincei, Rendic. Cl. Sci. Fis. Mat. Natur. **1975**, Ser.VIII, 54, 787-791.
- 11) Simonetta, M.; Gavezzotti, A.
Extended Hückel Investigation of Reaction Mechanism
In: *Structure and Bonding*, vol.27, Eds. Dunitz, J.D.; et al., Springer-Verlag, Berlin 1976, pp.1-43.
- Gavezzotti, A.
The 17 two-dimensional space groups: an illustration
Atti Accad. Naz. Lincei, Memorie Cl. Sci. Fis. Mat. Natur. **1976**, Ser. VIII, 13, 107-119.
- 12) Gavezzotti, A.; Simonetta, M.
Molecular Rearrangements in Organic Crystals. II. The Role of Intermolecular Cooperation
and Dipole-Dipole Interactions
Acta Crystallogr. **1976**, A32, 997-1001.
- 13) Gavezzotti, A.; Simonetta, M.
Extended Hückel Molecular Orbital Calculations for the Bridged Annulenes
Helv. Chim. Acta **1976**, 59, 2984-2998.
- Simonetta, M.; Gavezzotti, A.
Calculs Extended Hückel sur Molecules et Reactions Organiques
Bull.Soc.Chim.Belg. **1976**, 85, 947-952.
- 14) Gavezzotti, A.; Simonetta, M.
Extended Hückel study of the chemisorption of acetylene on the Pt(111) surface
Chem. Phys. Lett. 1977, 48, 434-438.
- Simonetta, M.; Gavezzotti, A.
Isomerizations and stereomutations in 1,2-dicyanocyclopropane. Extended Hückel calculations.
Atti della Accademia delle Scienze di Torino **1976-1977**, 111, 93-99.

- 15) Gavezzotti, A.; Simonetta, M.
The mechanism of organic reactions in the solid state. The rearrangement of *p*-dimethylaminobenzenesulfonate to *p*-trimethylammoniumbenzenesulfonate
Nouv. J. Chim. **1977**, *2*, 69-72.
- 16) Simonetta, M.; Gavezzotti, A.
General and Theoretical Aspects of the Acetylenic Compounds
In *The Chemistry of The Carbon-Carbon Triple Bond*, Ed.: S. Patai, Wiley, New York 1978, Cap. 1.
- 17) Destro, R.; Gavezzotti, A.; Simonetta, M.
Salicylideneaniline
Acta Crystallogr. **1978**, B34, 2867-2869.
- 18) Gavezzotti, A.; Simonetta, M.
EHT study of the dissociative chemisorption of acetylene on the Pt(111) surface
Chem. Phys. Lett. **1979**, *61*, 435-440.
- Simonetta, M.; Gavezzotti, A.
The Application of the Extended Hückel Method to Surface Chemistry and Crystals; acetylene on Pt(111)
Proceedings of the IV International Conference on Computers in Chemistry, Novosibirsk, 1979.
- 19) Gavezzotti, A.; Ortoleva, E.; Simonetta, M.
Extended Hückel Calculations on the Chemisorption of Acetylene on Tungsten
Theoret. Chim. Acta 1979, *52*, 209-218.
- 20) Gavezzotti, A.; Bartell, L.S.
Bond Orbitals and Intramolecular Interactions. 1. Barriers to Rotation and Nonbonded Interactions
J. Am. Chem. Soc. **1979**, *101*, 5142-5146.
- 21) Gavezzotti, A.; Simonetta, M.
The Chemisorption of Acetylene on the Pt(111) Surface. Extended Hückel Results
in: *Catalysis in Chemistry and Biochemistry. Theory and Experiment*, Ed.: B. Pullman, Reidel, Dordrecht 1979, pp. 241-253.
- 22) Gavezzotti, A.; Simonetta, M.
Structure and Reactivity: An Extended Hückel Approach
In: *Quantum Theory of Chemical Reactions*, Eds.: R. Daudel, A. Pullman, L. Salem and A. Veillard, Reidel, Dordrecht 1979, vol.I, pp.145-159,
- 23) Gavezzotti, A.; Simonetta, M.
An Extended Hückel study of adsorption of acetylene on Pt(111)
Surf. Sci. **1980**, *99*, 453-470.
- 24) Simonetta, M.; Gavezzotti, A.
General and Theoretical Aspects, In: *The Chemistry of the Sulphonium Group*, Eds.: C. J. M. Stirling and S. Patai, Wiley, New York 1981, cap.1.,
- 25) Simonetta, M.; Gavezzotti, A.
The Cluster Approach in Theoretical Study of Chemisorption. In: *Advances in Quantum Chemistry*, Ed.: P.-O. Lowdin, Academic Press, New York 1980, vol.12, pp.103-158.

- 26) Filippini, G.; Gavezzotti, A.; Simonetta, M.; Mason, R.
Lattice energies of crystals of n-alkanes: molecular motions, defects and phase transitions
Nouv. J. Chim. **1981**, *5*, 211-217.
- 27) Gavezzotti, A.; Ortoleva, E.; Simonetta, M.
Extended-Hückel Calculations on Chemisorption. Comparison of the Results for Acetylene
on Ni(111), Rh(111) and Pt(111) Surfaces
J. Chem. Soc. Faraday Trans. I **1982**, *78*, 425-436.
- 28) Gavezzotti, A.; Simonetta, M.
Crystal Chemistry in Organic Solids
Chem. Rev. **1982**, *82*, 1-13.
- 29) Destro, R.; Gavezzotti, A.; Simonetta, M.
syn-1,6-imino-8,13-methano[14]annulene
Acta Crystallogr. **1982**, *B38*, 1352-1354.
- 30) Gavezzotti, A.; Simonetta, M.
Determination of the orientation of naphthalene molecules on Pt(111) by packing energy calculations
Surf. Sci. **1982**, *116*, L207-L210.
- 31) Bartell, L.S.; Rothman, M.J.; Gavezzotti, A.
Pseudopotential SCF-MO studies of hypervalent compounds. IV. Structure, vibrational
assignments, and intramolecular forces in IF₇
J. Chem. Phys. **1982**, *76*, 4136-4143.
- 32) Gavezzotti, A.; Simonetta, M.; Van Hove, M.A.; Somorjai, G.A.
Force-field calculations of the packing energy of monolayers of C₃ and C₄ hydrocarbon
molecules adsorbed on single crystal metal surfaces
Surf. Sci. **1982**, *122*, 292-306.
- 33) Gavezzotti, A.
Calculations on packing energies, packing efficiencies and rotational freedom for molecular crystals
Nouv. J. Chim. **1982**, *6*, 443-450.
- 34) Gavezzotti, A.; Simonetta, M.
Force field calculations on the structure and energy of azulene layers on Pt(111)
Chem. Phys. Lett. **1982**, *92*, 16-18.
- 35) Gavezzotti, A.; Ortoleva, E.; Simonetta, M.
Extended Hückel studies of chemisorption on nickel. Substituted acetylenes and kink sites
Nouv. J. Chim. **1983**, *7*, 137-141.
- 36) Bartell, L.S.; Gavezzotti, A.;
Pseudopotential SCF-MO studies of hypervalent compounds. Part III. I₂, IF, IF₃ and IF₅
J. Mol. Struct. THEOCHEM **1983**, *91*, 331-336.
- 37) Beringhelli, T.; Filippini, G.; Gavezzotti, A.; Simonetta, M.
Packing analysis and sublimation energies of borane crystals
J. Mol. Struct. THEOCHEM **1983**, *94*, 51-61.

- 38) Gavezzotti, A.; Ortoleva, E.; Simonetta, M.
Naphthalene and azulene adsorption on Pt(111). Extended Hückel calculations
Chem. Phys. Lett. **1983**, *98*, 536-540.
- 39) Gavezzotti, A.
The Calculation of Molecular Volumes and the Use of Volume Analysis in the Investigation
of structured Media and of Solid-State Organic Reactivity
J. Am. Chem. Soc. **1983**, *105*, 5220-5225.
- 40) Gavezzotti, A.; Simonetta, M.
On the generation of trial structures and the evaluation of the formation energy for layers
of chemisorbed molecules on metal surfaces: naphthalene and azulene on Rh(111)
Surf. Sci. **1983**, *134*, 601-613.
- Gavezzotti, A.
Packing analysis for reactive crystals (Proceedings of Int. Conf. Chem. Organic Solid State, ICCOSS,
Freiburg i. B., 1982)
Mol. Cryst. Liq. Cryst. **1983**, *93*, 113-118.
- 41) Gavezzotti, A.; Tantardini, G.F.; Simonetta, M.
SCF-MO-pseudopotential studies of chemisorption. Hydrogen+Pt(111) clusters
Chem. Phys. **1984**, *84*, 453-461.
- 42) Bellezza, O.; Cattania, M.G.; Gavezzotti, A.; Simonetta, M.
SCF-MO-pseudopotential studies of chemisorption. The Pd(111)/oxygen system
Chem. Phys. Lett. **1984**, *108*, 425-429.
- Simonetta, M.; Gavezzotti, A.
Extended Hückel and empirical force field calculations for chemisorption on metal surfaces
Proceedings XIV Congr. Theoretical Chemists of Latin Expression, Louvain, 1983
J. Mol. Struct. THEOCHEM **1984**, *107*, 75-86.
- 43) Gavezzotti, A.
Molecular Free Surface: A Novel Method of Calculation and Its Uses in Conformational
Studies and in Organic Crystal Chemistry
J. Am. Chem. Soc. **1985**, *107*, 962-967.
- 44) Gavezzotti, A.; Simonetta, M.; van Hove, M.A.; Somorjai, G.A.
Adsorbate-adsorbate interactions and the ordering of organic monolayers on metal surfaces
Surf. Sci. **1985**, *154*, 109-120.
- Barone, V. Gavezzotti, A.; Russo, N.; Simonetta, M.
Superfici e Chemiadsorbimento: Calcoli Teorici con il Modello degli Aggregati
In *Problemi e metodi di scienza delle superfici*, Eds.: G.Del Re, N.Russo, Marra Editore,
Cosenza 1985.
- 45) Garfunkel, E.L.; Minot, C.; Gavezzotti, A.; Simonetta, M.
Benzene adsorption on the Rh(111) metal surface : a theoretical study
Surf. Sci. **1986**, *167*, 177-197.

- 46) Bianchi, R.; Gavezzotti, A.; Simonetta, M.
Molecular shape and crystal packing analysis of 11,11-disubstituted 1,6-methano[10]annulenes
J. Mol. Struct. THEOCHEM **1986**, *135*, 391-401.
- 47) Gavezzotti, A.; Simonetta, M.
On the symmetry of periodic structures in two dimensions
Computers and Mathematics with Applications **1986**, *12B*, 465-476.
- 48) Gavezzotti, A.; Bianchi, R.
Potential energy calculations and packing analysis for molecular motions in reactive diacyl peroxide crystals
Chem. Phys. Lett. **1986**, *128*, 295-299.
- 49) Gavezzotti, A.; Tantardini, G.F.; Simonetta, M.
SCF MO pseudopotential studies of chemisorption. The Pd(111)/CO system, with an optimized Pd pseudopotential
Chem. Phys. **1986**, *105*, 333-344.
- 50) Gavezzotti, A.; Tantardini, G.F.; Simonetta, M.
Molecular-Orbital calculations on Pt, PtH and PtCO with an optimized relativistic pseudopotential for Pt
Chem. Phys. Lett. **1986**, *129*, 577-581.
- 51) Gavezzotti, A.
Packing analysis in reactive crystals: the decomposition of bis(3,3,3-triphenylpropanoyl) peroxide in the solid state
Tetrahedron **1987**, *43*, 1241-1251.
- 52) Gavezzotti, A.; Simonetta, M.
Molecular Motion in Organic Crystals: the Structural Point of View
In *Organic Solid State Chemistry*, Ed.: G.R.Desiraju, Elsevier, Amsterdam 1987.
- 53) Destro, R.; Favini, G.; Gavezzotti, A.
Experimental and theoretical studies of organic molecules and crystals
Int. Revs. Phys. Chem. **1987**, *6*, 291-298.
- 54) Gavezzotti, A.
Theoretical Studies of Solid-State Reactivity by Packing Density and Potential-Energy Maps: Hydrogen Transfer in 5-Nitro-3-thiophenecarboxaldehyde Crystals
Acta Crystallogr. **1987**, *B43*, 559-562.
- 55) Gavezzotti, A.
General and Theoretical Aspects
In: *The Chemistry of Sulphones and Sulphoxides*, Eds.: S.Patai, Z.Rappoport and C.J.M.Stirling, Wiley, New York 1988, Cap. 1.
- 56) Gavezzotti, A.; Tantardini, G.F.; Miessner, H.
SCF-MO-Pseudopotential and Extended Hückel Calculations on the Interaction of CO with Pt Clusters
J. Phys. Chem. **1988**, *92*, 872-878. (M. Simonetta Special Issue)

57) Gavezzotti, A.; Simonetta, M.
The interaction between theoretical and crystallographic methods
Proceedings of the International Symposium on Molecular Structure, Beijing, 1986
In *Molecular Structure: Chemical Reactivity and Biological Activity*, Eds.: J.J.Stezowski, J.-L.Huang
and M.-C.Shao, International Union of Crystallography-Oxford University Press, Oxford 1988.

Gavezzotti, A.
Theoretical Studies of Molecular Motions and Reactivity in Organic Crystals
Proceedings of VIII Int. Conf. on the Chemistry of the Organic Solid State, Lyon, 1987
Mol. Cryst. Liq. Cryst. **1988**, 156, 25-33.

58) Gavezzotti, A.; Desiraju, G.R.
A Systematic Analysis of Packing Energies and Other Packing Parameters for Fused-Ring
Aromatic Hydrocarbons
Acta Crystallogr. **1988**, B44, 427-434.

Gavezzotti, A.
Crystal packing modes of hydrocarbons. Statistics on all the available crystal structures in the
Cambridge Data Files
Proceedings of the XI European Crystallographic Meeting, Vienna, 1988
Z. Krist. **1988**, 185, 717

59) Gavezzotti, A.
Statistical Analysis of Some Structural Properties of Solid Hydrocarbons
J. Am. Chem. Soc. **1989**, 111, 1835-1843.

60) Desiraju, G.R.; Gavezzotti, A.
From Molecular to Crystal structure; Polynuclear Aromatic Hydrocarbons
J. Chem. Soc. Chem. Commun. 1989, 621-623.

61) Desiraju, G.R.; Gavezzotti, A.
Crystal Structure of Polynuclear Aromatic Hydrocarbons. Classification, Rationalization
and Prediction from Molecular Structure
Acta Crystallogr. **1989**, B45, 473-482.

Gavezzotti, A.
Molecular Shape and Crystal Packing Modes for Organic Molecules: a Computational Approach
Proceedings of OMNO Conference, Oxford 1988
In *Organic Materials for Non-linear Optics*, Eds.: R.A.Hann and D.Bloor, Special Publ.N.69,
The Royal Society of Chemistry, London 1989.

62) Gavezzotti, A.;
On the preferred mutual orientation of aromatic groups in organic condensed media
Chem. Phys. Lett. **1989**, 161, 67-72.

63) Gavezzotti, A.;
Crystal Packing of Hydrocarbons. Effects of Molecular Size, Shape and Stoichiometry
Acta Crystallogr. **1990**, B46, 275-283.

- 64) Gavezzotti, A.;
Packing Analysis of Organic Crystals Containing C=O or C≡N Groups
J. Phys. Chem. **1990**, *94*, 4319-4325.
- 65) Destro, R.; Gavezzotti, A.
Intermolecular Energies and Packing Modes in Organic Crystals
In: *Structure and Properties of Molecular Crystals*, Ed.: M.Pierrot, Elsevier, Amsterdam 1990,
Chapter 3, pp. 161-210.
- Gavezzotti, A.
The prediction of the crystal packing of organic molecules: geometry and intermolecular potentials
Proceedings of a NATO Advanced Workshop, Erice, 1990
In: *Electron Crystallography of Organic Molecules*, Eds.: J.R.Fryer and D.L.Dorset, Kluwer, 1990, pp.77-83.
- 66) Bernstein, J.; Sarma, J.A.R.P ; Gavezzotti, A.
Generation of unknown crystal phases for aromatic hydrocarbons by packing energy calculations
Chem. Phys. Lett. **1990**, *174*, 361-368.
- 67) Gavezzotti, A.; Filippini, G.
Crystal packings and lattice energies of polythienyls: calculations and predictions
Synth. Metals **1991**, *40*, 257-266.
- 68) Gavezzotti, A.
Generation of Possible Crystal Structures from the Molecular Structure for Low-Polarity Organic Compounds
J. Am. Chem. Soc. **1991**, *113*, 4622-4629.
- 69) Gavezzotti, A.
Molecular Packing and Other Structural Properties of Crystalline Oxohydrocarbons
J. Phys. Chem. **1991**, *95*, 8948-8955.
- 70) Braga, D.; Grepioni, F.; Sabatino, P.; Gavezzotti, A.
Molecular Organization in Crystalline [Co₂(CO)₈] and [Fe₂(CO)₉] and a Search for Alternative Packings for [Co₂(CO)₈]
J. Chem. Soc. Dalton Trans. **1992**, 1185-1191.
- 71) Filippini, G.; Gavezzotti, A.
A Quantitative Analysis of the Relative Importance of Symmetry Operators in Organic Molecular Crystals
Acta Crystallogr. **1992**, *B48*, 230-234.
- 72) Gavezzotti, A.; Filippini, G.
Molecular packing of crystalline azahydrocarbons
Acta Crystallogr. **1992**, *B48*, 537-545.
- Filippini, G.; Gavezzotti, A.
Crystal structure versus molecular structure: New developments
Proceedings International Conference on the Chemistry of the organic Solid State, Como 1991
Mol. Cryst. Liquid Cryst. **1992**, *219*, 37-41.

- 73) Simonetta, M.; Gavezzotti, A.
Structural Chemistry
In: *Accurate molecular structures*, Eds.: A.Domenicano, I.Hargittai, International Union of Crystallography-Oxford University Press, Oxford 1992, Chapter 1.
- 74) Filippini, G.; Gavezzotti, A.
Empirical intermolecular potentials for organic crystals: the 6-exp approximation revisited
Acta Crystallogr. **1993**, *B49*, 868-880.
- 75) Gavezzotti, A.; Filippini, G.
The Crystal Packing of Chlorine- and Sulfur-containing Compounds
Acta Chimica Hungarica - Models in Chemistry **1993**, *130*, 205-220.
- Gavezzotti, A.; Filippini, G.
Possible Control and Prediction of Crystal Structure: Optimized Potential Functions for non-Hydrogen Bonded Organic Crystals
Proceedings ?
Mol. Cryst. Liq. Cryst. **1993**, *235*, 225-230.
- 76) Bock, H.; Goebel, I.; Naether, C.; Havlas, Z.; Gavezzotti, A.; Filippini, G.
Monoclinic and Triclinic Tetraisopropyl-*p*-phenylenediamine:
To what Extent do n/π Interactions Determine Structures?
Angew.Chem. **1993**, *105*, 1823-1826; *Angew.Chem.Int.Ed.* **1993**, *32*, 1755-1758.
- 77) Gavezzotti, A.
Molecular packing and correlations between molecular and crystal properties
in *Structure Correlation*, Eds.: H.B.Burgi, Dunitz, J.D.; VCH, Weinheim 1994, vol. 2, pp. 509-542.
- 78) Gavezzotti, A.; Filippini, G.
Geometry of the Intermolecular X-H...Y (X,Y=N,O) Hydrogen Bond, and the Calibration of Empirical Hydrogen-Bond Parameters
J. Phys. Chem. **1994**, *98*, 4831-4837.
- Gavezzotti, A.; Filippini, G.
Non-covalent interactions in organic crystals, and the calibration of empirical force fields
In: *Computational Approaches to Supramolecular Chemistry*, Ed.: G.Wipff, Kluwer, Dordrecht 1994, pp.51-62
- 79) Gavezzotti, A.
Are crystal structures predictable?
Acc. Chem. Res. **1994**, *27*, 309-314
- 80) Filippini, G.; Gavezzotti, A.
The crystal structure of 1,3,5-triamino-2,4,6-trinitrobenzene. Centrosymmetric or non-centrosymmetric?
Chem. Phys. Lett. **1994**, *231*, 86-92.
- 81) Bock, H.; Rauschenbach, A.; Naether, C.; Havlas, Z.; Gavezzotti, A.; Filippini, G.
Orthorhombic and monoclinic 2,3,7,8-tetramethoxythianthrene: small structural difference-large lattice change
Angew.Chem.Int.Ed.Engl. **1995**, *34*, 76-78; *Angew. Chem.* **1995**, *107*, 120-122.

- 82) Gavezzotti, A.
Molecular symmetry, melting temperatures and melting enthalpies of substituted benzenes and naphthalenes
J. Chem. Soc. Perkin 2 **1995**, 1399-1404.
- 83) Gavezzotti, A.; Filippini, G.
Polymorphic forms of organic crystals at room conditions: thermodynamic and structural implications
J. Am. Chem. Soc. **1995**, *117*, 12299-12305.
- 84) Gavezzotti, A.
Polymorphism of 7-dimethylaminocyclopenta(c)coumarin: packing analysis and generation of trial structures
Acta Crystallogr. **1996**, *B52*, 201-208.
- 85) Gavezzotti, A.; Filippini, G.
Computer prediction of organic crystal structures using partial X-ray diffraction data
J. Am. Chem. Soc. **1996**, *118*, 7153-7157.
- 86) Gavezzotti, A.
Organic crystals: engineering and design
Current Opinion in Solid state and material science, Eds.:A.K.Cheetham, H.Inokuchi, J.M.Thomas, **1996**, *1*, 501-505
- 87) Gavezzotti, A.
Crystal symmetry and molecular recognition
In: *Theoretical aspects and computer modeling of the molecular solid state*,
Ed.: A. Gavezzotti, Wiley and Sons, Chichester 1997, Chapter 1.
- 88) Gavezzotti, A.; Filippini, G.
Energetic aspects of crystal packing: experiment and computer simulations
In: *Theoretical aspects and computer modeling of the molecular solid state*,
Ed.: A. Gavezzotti, Wiley and Sons, Chichester 1997, Chapter 3.
- 89) Gavezzotti, A.; Filippini, G.; Kroon, J.; van Eijck, B.P.; Klewinghaus, P.
The crystal polymorphism of tetrolic acid: molecular dynamics study of precursors in solution, and a crystal structure generation
Chem. Eur. J. **1997**, *3*, 893-899.
- 90) Gavezzotti, A.
Computer simulations of organic solids and their liquid state precursors
Faraday Discuss. **1997**, *106*, 63-77
- 91) Gavezzotti, A.; Filippini, G.
Self-organization of small organic molecules in liquids, solutions and crystals: static and dynamic calculations
Chem. Commun. Feature Article **1998**, 287-294

- 92) Gavezzotti, A.
The crystal packing of organic molecules: challenge and fascination below 1000 dalton
Crystallography Reviews **1998**, 7, 5-121.
- 93) Gavezzotti, A.
Molecular aggregation of acetic acid in a carbon tetrachloride solution: a molecular dynamics study with a view to crystal nucleation
Chem. Eur. J. 1999, 5, 567-576.
- Gavezzotti, A.; Filippini, G.
Self-organization in molecular crystals, liquids and solutions: computer studies
In: *Current challenges in large supramolecular assemblies*, Ed.: G.Tsoucaris, Kluwer, Dordrecht 1999, pp.249-263.
- Gavezzotti, A.; Filippini, G.
The computer prediction of the assembling of organic molecules into crystals: a perspective
In: *Supramolecular engineering of synthetic metallic materials: conductors and magnets*, Ed.: J.Veciana, Kluwer, Dordrecht 1999, pp.41-51.
- Gavezzotti, A.
Methods and current trends in the simulation and prediction of organic crystal structures
Nova Acta Leopoldina **1999**, NF79, 33-46.
- 94) Dunitz, J.D.; Gavezzotti, A.
Attractions and repulsions in organic crystals: what can be learned from the crystal structures of condensed-ring aromatic hydrocarbons?
Acc. Chem. Res. **1999**, 32, 677-684.
- 95) Filippini, G.; Gavezzotti, A.; Novoa, J.J.
Modeling the crystal structure of 2-hydro nitronyl nitroxide radical (HNN): observed and computer-generated polymorphs
Acta Crystallogr. **1999**, B55, 543-553.
- 96) Gavezzotti, A.
A molecular dynamics view of some kinetic and structural aspects of melting in the acetic acid crystal
J. Mol. Struct. **1999**, 485-486,485-499 (L.S.Bartell Special Issue)
- Gavezzotti, A.
Molecular packing in liquids, solutions and crystals: acetic acid as a test case
In: *Crystal engineering: from molecules and crystals to materials*, Ed.: D.Braga, Kluwer, Dordrecht 1999, pp. 129-142.
- Gavezzotti, A.; Filippini, G.
Atom-atom empirical potentials for the static and dynamic simulation of condensed phases
In: *Advances in the computer simulation of liquid crystals*, Eds.: C.Zannoni, P.Pasini, Kluwer, Dordrecht 2000, pp. 235-250.
- 97) Gavezzotti, A.
A molecular dynamics study of the structure and evolution of the 4,4'-bis(diphenylhydroxymethyl)biphenyl/acetone host-guest system
Chem. Eur. J. **2000**, 6, 2288-2294

98) Lommerse, J.P.M.; Motherwell, W.D.S.; Ammon, H.L.; Dunitz, J.D.; Gavezzotti, A.; Hofmann, D.W.M.; Leusen, F.J.J.; Mooij, W.T.M.; Price, S.L.; Schweizer, B.; Schmidt, M.U.; van Eijck, B.P.; Verwer, P.; Williams D.E.

A test of crystal structure prediction of small organic molecules
Acta Crystallogr. **2000**, *B56*, 697-714.

99) Gavezzotti, A.

A molecular dynamics test of the different stability of crystal polymorphs under thermal strain
J. Am. Chem. Soc. **2000**, *122*, 10724-10725

100) Dunitz, J.D.; Filippini, G.; Gavezzotti, A.

A statistical study of density and packing variations among crystalline isomers
Tetrahedron **2000**, *56*, 6595-6601.

101) Dunitz, J.D.; Filippini, G.; Gavezzotti, A.

Molecular shape and crystal packing: a study of C₁₂H₁₂ isomers, real and imaginary
Helv. Chim. Acta **2000**, *83*, 2317-2335. (Albert Eschenmoser Special Issue)

102) Boese, R.; Kirchner, M.T.; Dunitz, J.D.; Filippini, G.; Gavezzotti, A.

Solid-stat behaviour of the dichlorobenzenes: actual, semi-virtual and virtual crystallography
Helv. Chim. Acta **2001**, *84*, 1561-1577. (Edgar Heilbronner Special Issue)

103) Gavezzotti, A.

The Chemistry of Intermolecular Bonding: Organic Crystals, their Structures and Transformations
Synthetic Letters **2002**, pp. 201-214.

104) Gavezzotti, A.

Structure and Intermolecular Potentials in Molecular Crystals
Modelling Simul. Mater. Sci. Eng. **2002**, *10*, R1-R29.

105) Motherwell, W.D. S.; Ammon, H. L.; Dunitz, J. D.; Dzyabchenko, A.; Erk, P.; Gavezzotti, A.; Hofmann, D. W.M.; Leusen, F.J.J.; Lommerse, J. P.M.; Mooij, W.T.M.; Price, S.L.; Scheraga, H.; Schweizer, B.; Schmidt, M. U.; van Eijck, B.P.; Verwer, P.; Williams, D. E.

Crystal Structure Prediction of Small Organic Molecules: a Second Blind Test
Acta Crystallogr. **2002**, *B58*, 647-661.

106) Gavezzotti, A.

The calculation of intermolecular interaction energies by direct numerical integration over electron densities. I Electrostatic and polarization energies in molecular crystals
J. Phys. Chem. **2002**, *B106*, 4145-4154.

107) Ferretti, V.; Gilli, P.; Gavezzotti, A.

X-ray diffraction and molecular simulation study of the crystalline and liquid state of succinic anhydride
Chem. Eur. J. **2002**, *8*, 1710-1718.

108) Gavezzotti, A.

Modeling Hydrogen bonded crystals
J. Mol. Struct. **2002**, *615*, 5-12.

- 109) Gavezzotti, A.; Dunitz, J.D.
Electrostatic energies in the 1,4-dichlorobenzene polymorph crystals: the role of charge density overlap effects in crystal packing analysis
Helv. Chim. Acta **2002**, *85*, 3949-3964. (D.Seebach Special Issue)
- 110) Gavezzotti, A.
Ten years of experience in polymorph prediction: what next?
Proceedings of CrystEngComm Discussion, Bristol, 2002)
CrystEng Comm. **2002**, *4*, 343-347.
- 111) Gavezzotti, A.
Calculation of intermolecular interaction energies by direct numerical integration over electron densities. 2. An improved polarization model and the evaluation of dispersion and repulsion energies
J. Phys. Chem. **2003**, *B107*, 2344-2353.
- 112) Destri, S.; Pasini, M.; Porzio, W.; Gavezzotti, A.; Filippini, G.
X-ray diffraction studies and computer simulations of the crystal and molecular structure of 2,5-di-(9,9-dimethylfluoren-2-yl)-3,4-dihexyl-thiophene-1,1-dioxide, a photoluminescent material
Cryst. Growth Des. **2003**, *3*, 257-262.
- 113) Boese, R.; Clark, T.; Gavezzotti, A.
Co-crystallization with acetylene. The 1:1 complex with benzene: crystal growth, X-ray diffraction and molecular simulations
Helv. Chim. Acta **2003**, *86*, 1085-1100 (J.D.Dunitz Special Issue)
- 114) Gavezzotti, A.
Towards a realistic model for the quantitative evaluation of intermolecular potentials and for the rationalization of organic crystal structures. I. Philosophy
CrystEngComm 2003, *5*, 429-438
- 115) Gavezzotti, A.
Towards a realistic model for the quantitative evaluation of intermolecular potentials and for the rationalization of organic crystal structures. II. Crystal energy landscapes
CrystEngComm 2003, *5*, 439-446
- Gavezzotti, A.
Structural, energetic and nucleation factors in the theoretical prediction of crystal structures for organic compounds
In.: *Proceedings of the Joint italo-french meeting on Crystal growth: from basic to applied*, Eds.: S.Carrà, C.Paorici, Accademia Nazionale dei Lincei, Roma 2003, pp. 31-45.
- 116) Dunitz, J.D.; Gavezzotti, A.
Molecular shape and intermolecular liaison: hydrocarbons and fluorocarbons
Helv. Chim. Acta **2003**, *86*,4073-4092 (Duilio Arigoni Special Issue)
- 117) Demartin, F.; Filippini, G.; Gavezzotti, A.; Rizzato S.
X-ray diffraction and packing analysis on vintage crystals: Wilhelm Koerner's nitrobenzene derivatives from the School of Agricultural Sciences in Milano
Acta Crystallogr. **2004**, *B60*, 609-620.
- Gavezzotti, A.
Cento biglie alla rinfusa
In: *Il ritmo delle forme*, Eds.: P.Bellingeri, M.Dedò, S.DiSieno, C.Turrini, Mimesi, Milano 2004, pp.113-120.

- 118) Dunitz, J.D.; Gavezzotti, A.
Intermolecular recognition and adhesion in organic crystals: directed intermolecular bonds or nonlocalized bonding?
Angew. Chem. Int. Ed. **2005**, *44*, 1766-1787.
- 119) Carlucci, L.; Gavezzotti, A.
Molecular recognition and crystal energy landscapes: an Xray and computational study of caffeine and other methylxanthines
Chem. Eur. J. **2005**, *11*, 271-279.
- 120) Gavezzotti, A.
Hierarchies of Intermolecular Potentials and Forces: Progress towards a Quantitative Evaluation
Structural Chemistry **2005**, *16*, 177-185.
- 121) Gavezzotti, A.
Calculation of lattice energies of organic crystals: the PIXEL integration method in comparison with more traditional methods
Z. Krist. **2005**, *220*, 499-510.
- Gavezzotti, A.; Flack, H.
Crystal Packing; Illustrations of the two-dimensional space groups
International Union of Crystallography Teaching Pamphlet n.21
International Union of Crystallography, 2005
<http://ww1.iucr.org/comm/cteach/pamphlets.html>
- 122) Gavezzotti, A.
Quantitative ranking of crystal packing modes by systematic calculations on potential energies and vibrational amplitudes of molecular dimers,
J. Chem. Theor. Comp. **2005**, *1*, 834-840.
- 123) Dunitz, J.D.; Gavezzotti, A.
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-thiphenecarbonitrile
Cryst. Growth Des. **2005**, *5*, 2180-2189.
- 124) Bacchi, S.; Benaglia, M.; Cozzi, F.; Demartin, F.; Filippini, G.; Gavezzotti, A.
X-ray diffraction and theoretical studies for the quantitative assessment of intermolecular arene-perfluoroarene stacking interactions
Chem. Eur. J. **2006**, *12*, 3538-3546.
- 125) Ferrari, E.S.; Burton, R.C.; Davey, R.J.; Gavezzotti, A.
Simulation of phase separation in alcohol/water mixtures using two-body force field and standard molecular dynamics
J. Comp. Chem. **2006**, *27*, 1211-1219.
- 126) Gavezzotti, A.
Supramolecular interactions: energetic considerations
In: *Making crystals by design*, Eds.: D.Braga, F.Grepioni, Wiley-VCH, Weinheim 2006, Chapter 1.

Gavezzotti, A.

The Pixel module of the OPiX computer program package: affordable calculation of intermolecular interaction energies for large organic molecules and crystals

In: Newsletter nov. 2006, International Union of Crystallography, Commission for Crystallographic Computing (Chair: A.L.Spek), pp. 45-58.

<http://www.iucr.org/resources/commissions/crystallographic-computing/newsletters/7>

127) Gavezzotti, A.; C.J.Eckhardt

Computer simulation and analysis of structural and energetic features of some crystalline energetic materials

J. Phys. Chem. **2007**, *B111*, 3430-3437

128) Gavezzotti, A.

A solid-state chemist's view of the crystal polymorphism of organic compounds

J. Pharm. Sci. **2007**, *96*, 2232-2241

129) Cozzi, F.; Bacchi, S.; Filippini, G.; Pilati, T.; Gavezzotti, A.

Synthesis, X-ray diffraction, and computational study of the crystal packing of some polycyclic hydrocarbons featuring aromatic and perfluoroaromatic rings condensed in the same molecule:

1,2,3,4-tetrafluoronaphthalene, 1,2,3,4-tetrafluoroanthracene and 1,2,3,4-tetrafluorophenanthrene
Chem. Eur. J. **2007**, *13*, 7177-7184

Dunitz, J.D.; Gavezzotti, A.

Molecular cohesion and the structure of organic crystals

In: *Turning Points in Solid-State, Materials and Surface Science*, Eds.: K.D.M.Harris and P.P.Edwards, Royal Society of Chemistry Publishing, London 2007, Ch.18

130) Gavezzotti, A.

Structure and energy in organic crystals with two molecules in the asymmetric unit: causality or chance?

CrystEngComm **2008**, *10*, 389-398.

131) Bernstein, J.; Dunitz, J.D.; Gavezzotti, A.

Polymorphic perversity: crystal structures with many symmetry-independent molecules in the unit cell
Cryst. Growth Des. **2008**, *8*, 2011-2018.

132) Gavezzotti, A.

Hydrogen bond strength and bond geometry in cyclic dimers of crystalline carboxylic acids

Acta Crystallogr. **2008**, *B64*, 401-403.

133) Gavezzotti, A.

Non-conventional bonding between organic molecules. The 'halogen bond' in crystalline systems

Mol. Phys. **2008**, *106*, 1473-1485 (A.J.Stone Special Issue)

134) Gavezzotti, A.

Coulombic and dispersive factors in the molecular recognition of peptides: PIXEL calculations on two NNQQ (Asn-Asn-Gln-Gln) crystal polymorphs

Acta Crystallogr. **2008**, *D64*, 905-908.

Gavezzotti, A.

Forty years of struggle with computers over crystallography and intermolecular interactions

ACA Reflexions, no.1, pp. 22-23, American Crystallographic Association Buffalo 2008.

- 135) Gibson, E.K.; Winfield, J.M.; Muir, K.W.; Carr, R.H.; Eaglesham, A.; Gavezzotti, A.; Parker, S.F.; Lennon, D.
A structural and spectroscopic investigation of the hydrochlorination of 4-benzylaniline: the interaction of anhydrous hydrogen chloride with chlorobenzenes
Phys. Chem. Chem. Phys. **2009**, *11*, 288-297.
- 136) Cozzi, F.; Bacchi, S.; Filippini, G.; Pilati, T.; Gavezzotti, A.
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
CrystEngComm **2009**, *11*, 1122-1127.
- 137) J.D.Dunitz, A.Gavezzotti
How molecules stick together in organic crystals: weak intermolecular interactions
Chem.Soc.Revs. **2009**, *38*, 2622-2633
- 138) Gibson, E.K.; Winfield, J.M.; Muir, K.W.; Carr, R.H.; Eaglesham, A.; Gavezzotti, Lennon, D.
A structural and spectroscopic investigation of the hydrochlorination of 4,4'-methylenedianiline
Phys. Chem. Chem. Phys. **2010**, *12*, 3824-3833.
- 139) Gavezzotti, A.
Normalized one- and two-dimensional distribution functions for interatomic distance and angle data from crystallographic databases
J. Appl. Cryst. **2010**, *43*, 429-433
- 140) Gavezzotti, A.
The lines-of-force landscape of interactions between molecules in crystals. Cohesive *versus* tolerant and "collateral damage" contact
Acta Crystallogr. **2010**, *B66*, 396-406
- 141) Gavezzotti, A.
Can a computer crystallize a liquid? Molecular simulation of continuous trajectories from liquid to crystalline n-hexane
CrystEngComm **2011**, *13*, 3573-3579
- 142) Gavezzotti, A.
Efficient computer modeling of organic materials. The atom-atom, Coulomb-London-Pauli (AA-CLP) model for intermolecular electrostatic-polarization, dispersion and repulsion energies
New J. Chem. **2011**, *35*, 1360-1368
- 143) Maschio, L.; Civalleri, B.; Ugliengo, P.; Gavezzotti, A.
Intermolecular interaction energies in organic crystals: comparison and agreement of Localized Moeller-Plesset 2, dispersion-corrected density functional, and classical empirical two-body calculations
J. Phys. Chem. **A2011**, *115*, 11179-11186.
- 144) Gavezzotti, A.
Computational studies of crystal structure and bonding, in "Advanced X-ray Crystallography" (Topics in Current Chemistry), Ed. K.Rissanen, Springer-Verlag, Berlin 2011.
- 145) Gavezzotti, A.; Dunitz, J.D.
Proteogenic amino acids: chiral and racemic crystal packings and stabilities
J. Phys. Chem. B, **2012**, *116*, 6740-6750.

- 146) Gavezzotti, A; Demartin, F.; Castellano, C.; Campostrini, I.
Polymorphism of As₄S₃, (tris-(μ₂-sulfido)-tetra-arsenic). Accurate structure refinement on natural α- and β-dimorphites and inferred thermodynamic properties.
Phys.Chem. Minerals **2013**, *40*, 175-182
- 147) Dunitz, J. D.; Gavezzotti, A.
Supramolecular synthons: validation and ranking of intermolecular interaction energies
Cryst. Growth Des. **2012**, *12*, 5873-5877
- 148) Gavezzotti, A.
The "sceptical chymist": intermolecular doubts and paradoxes
CrystEngComm Highlight, **2013**, *15*, 4027-4035
- 149) Gavezzotti, A.
Equilibrium structure and dynamics in organic crystals by Monte Carlo simulation. Critical assessment of force field and comparison with static packing analysis
New J. Chem. **2013**, *37*, 2110-2119
- 150) Gavezzotti, A.
Crystal formation and stability: physical principles and molecular simulation
Cryst.Res.Technol.**2013**, *48*, 793-810.
- 151) Gavezzotti, A.
Molecular level insights on the liquid-solid transition of large organics by biased Monte Carlo simulation
Cryst. Growth Des. **2013**, *13*, 3801-3815
- 152) Dunitz J.D.; Gavezzotti, A.; Rizzato, S.
"Coulombic compression", a pervasive force in ionic solids. A study of anion stacking in croconate crystals
Cryst. Growth Des. **2014**, *14*, 357-366
- 153) Gavezzotti, A.; Rizzato, S.
Are racemic crystals favored over homochiral crystals by higher stability or by kinetics? Insights from comparative studies of crystalline stereoisomers
J. Org. Chem. **2014**, *78*, 4909-4916
- 154) Gavezzotti, A.; Lo Presti, L.
Theoretical study of chiral carboxylic acids. Structural and energetic aspects of crystalline and liquid states
Cryst. Growth Des. **2015**, *15*, 3792-3803
- 155) Gavezzotti, A.
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 J. Chem. **2016**, *40*, 6848-6853
- 156) Gavezzotti, A.; Colombo, V.; LoPresti, L.
Facts and factors in the formation and stability of binary crystals
Cryst. Growth Des. **2016**, *16*, 6095-6104

- 157) Fabbiani, F.P.A.; Bergantin, S.; Gavezzotti, A.; Rizzato, S.; Moret, M.
X-ray diffraction and computational studies of the pressure-dependent tetrachloroethane solvation of diphenylanthracene
CrystEngComm **2016**, 18, 2173-2181.
- 158) Gavezzotti, A.; Lo Presti, L.
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
Cryst. Growth Des. **2016**, 16, 2952-2962
- 159) Gavezzotti, A.
Topics in structural chemistry through after dinner humor
Isr. J. Chem. **2017**, 57, 13-23
- 160) Braga, D.; Grepioni, F.; Gavezzotti, A.; Bernstein, J.
Re: Crystal engineering in the regulatory and patent literature of pharmaceutical forms
Cryst. Growth Des. **2017**, 17, 933-939
- 161) Colombo, V. Lo Presti, L.; Gavezzotti, A.
Two-component organic crystals without hydrogen bonding: structure and intermolecular interactions in bimolecular stacking
CrystEngComm **2017**, 19, 2415-2423
- 162) Carlucci, L.; Gavezzotti, A.
A quantitative measure of halogen bond activation in cocrystallization
Chem.Phys.Phys.Chem. **2017**, 19, 18383-18388
- 163) Gavezzotti, A.
Bonding in organic molecules and condensed phases. The role of repulsions
In *Intermolecular Interactions in Crystals: Fundamentals of Crystal Engineering*
Edited by Juan J. Novoa, Royal Society of Chemistry, 2017.
- 164) Gavezzotti, A.
Pillars of crystal engineering: crystal energies and symmetry operators
CrystEngComm **2018**, 20, 2511-2518

Books

- Gavezzotti, A.
Cinetica chimica con esperimenti e problemi
Editrice Scientifica L.Guadagni, Milano 1982.
- Gavezzotti, A.
Principi di chimica Fisica
Casa Editrice Ambrosiana, Milano 1993
- Gavezzotti, A.
Molecular aggregation, Structure analysis and molecular simulation of crystals and liquids
Oxford University Press, Oxford 2007; 2nd Edition paperback, 2013
- Gavezzotti, A.
An Introduction to Physical Chemistry, The structural approach
Aracne Editrice, Roma 2008