Angelo Gavezzotti

Lectures and seminars

1) **19.6.1980** Istituto di Chimica Industriale, Universita' di Genova (Italy)
Orbitali legame e interazioni intermolecolari

2) **16.11.1981** Surface science and catalysis seminar, MMRD-Lawrence Berkeley Laboratory, Berkeley (USA)
Quantum chemical and force-field calculations on chemisorption

3) **24.11.1982** Laboratoire de Chimie Industrielle, Universite' Claude Bernard, Lyon (France)
Packing analysis in organic crystals

4) **8.9.1983** Scuola dell'Associazione Italiana di Cristallografia su Metodi interpretativi delle geometrie molecolari, Perugia (Italy)
Meccanica molecolare

5) **20.10.1983** Surface science and catalysis seminar, MMRD-Lawrence Berkeley Laboratory, Berkeley (USA)
Generation of trial structures and evaluation of formation energies for layers of molecules

6) **16.12.1983** Institut de Chimie Moleculaire d'Orsay, Universite' Paris-sud (France)
Semiempirical calculations on bonding between transition metals and hydrocarbons

7) **22.11.1984** Istituto di Chimica Fisica, Universita' di Parma (Italy)
Aspetti teorici del legame chimico tra metalli di transizione e composti covalenti

8) **5.9.1985** Mycrosymposium on Elementary Processes and Chemical Reactivity, Liblice (Czechoslovakia)
Quantum chemical and force-field calculations on chemisorpion on metal surfaces

9) **16.1.1986** EuChem Congress on Molecular Materials for Electronics and Optoelectronics, Les Arcs (France)
Organic solid state

10) **1.4.1986** Seminaire Mecanismes de la Catalyse Heterogene, Universite' Lyon I (France)
Molecular orbital calculations on chemisorption: feasibility and reliability

11) **24.5.1986** Akademie der Wissenschaften der DDR, Berlin;
12) **28.5.1986** Friedrich-Schiller Universitat, Jena (DDR)
Quantum chemical calculations on chemisorption

13) **16.9.1986** International Symposium on Molecular Structure, Beijing (P.R.China)
The interaction between theoretical and crystallographic methods

14) **14.10.1986** Institut fur Physikalische Chemie, Universität Innsbruck (Austria)
Molecular orbital and semiempirical calculations on chemisorption

15) **25.11.1986** Societa' Chimica Italiana at Universita' di Milano (Italy)
Analisi dell'impaccamento e del moto molecolare in cristalli organici

16) **11.3.1987** Laboratorium fur Organische Chemie, ETH, Zürich (Switzerland)
Theoretical and crystallographic studies on the packing of organic molecules in crystals

17) **9.7.1987**, VIII International Congress on the Chemistry of the Organic Solid State, Lyon (France)
A theoretical approach to the study of organic solid state reactions

18) **22.10.1987** First Italian-Israeli meeting, The influence of steric and electronic effects on molecular crystalline structure, Firenze (Italy)
Molecular shape and packing analysis for organic crystals

19) **21.3.1988** Faculte' de Sciences, Universite' de Marseille (France)
Statistical analysis of molecular properties and molecular packing in organic crystals

20) **29.4.1988** Laboratorium für Chemische und Mineralogische Kristallographie, Universität Bern (Switzerland)
Statistical analysis of molecular packing properties in organic crystals

21) **30.6.1988** International Conference on Organic Materials for Non-linear Optics, University of Oxford (UK)
Molecular shape and crystal packing modes for organic molecules: a computational approach

22) **5.9.1989** Inorganic Chemistry Laboratory, University of Oxford (UK)
Packing geometries and packing forces in organic crystals

23) **13.9.1989** Scuola Associazione Italiana di Cristallografia su Forze di interazione nei cristalli, Perugia (Italy)
Correlazione tra struttura molecolare e struttura cristallina

24) **22.2.1990** Mendel D.Cohen Memorial Symposium, The Weizmann Institute of Science, Rehovot (Israel)
The crystal packing of organic molecules: prediction from molecular structure

25) **15.3.1990** Symposium in honor of J.D.Dunitz, Swiss Crystallographic Association, ETH, Zürich (Switzerland)
The crystal packing of organic molecules: geometry and forces

26) **23.4.1990** NATO ARW on Electron Crystallography, Ettore Majorana Centre, Erice (Italy)
The crystal packing of organic molecules: geometry and intermolecular potentials

27) **14.5.1990** BASF-AG, Ludwigshafen (Germany)
Control and prediction of organic crystal packing. State of the art

28) **4.6.1991** International School of Crystallography, Ettore Majorana Centre, Erice (Italy)
Modern uses of packing energy calculations

29) **10.9.1991** Scuola dell'Associazione Italiana di Cristallografia, Perugia (Italy)
Aspetti termodinamici dei cristalli organici

30) **18.9.1991** Institut Laue-Langevin, Grenoble (France)
Control and prediction of crystal structure for organic compounds. State of the art and perspectives

31) **28.10.1991** International Symposium on Analysis and Control of Reactions in Molecular Crystals, Tokyo Institute of Technology, Tokyo (Japan)
Intermolecular potential in organic and organometallic crystals: static and dynamic aspects

32) **30.10.1991** Mitsubishi-Kasei Company, Yokohama (Japan)
Molecular interactions and crystal packing

33) **1.11.1991** Toyohashi University of Technology, Toyohashi (Japan)
Relationship between molecular and crystal structure for organic compounds

34) **3.2.1992** Second Italian-Israeli Symposium, The influence of steric and electronic effects on molecular and crystalline structure, Herzlyia (Israel)
New empirical potential functions for non-hydrogen bonded organic crystals

35) **13.2.1992** Annual meeting of the Israel Chemical Society, Haifa (Israel)
Intermolecular potentials in organic crystals: new developments

36) **19-23.10.1992** University of Barcelona (Spain)
Course on crystal packing (10 hours)

37) **3.9.1993** NATO ARW: Computational approaches in supramolecular chemistry, Strasbourg (France)
Non-covalent interactions in crystals

38) **March 1994** Glaxo Company, Verona (Italy)
Metodi diffrattometrici per la chimica strutturale: tecniche a raggi X

39) **28.2.1994**, Max-Planck Institut fur Festkorperforschung, Stuttgart (Germany)
40) **1.3.1994** Max-Planck Institut fur Kohlenforschung, Mulheim (Germany)
41) **3.3.1994**, Institut fur Anorganische Chemie, Universitat Frankfurt (Germany)
42) **4.3.1994**, University of Heidelberg (Germany)
Molecular crystal structures: to what extent can they be predicted?

43) **4.3.1994** BASF-AG, Ludwigshafen (Germany
Molecular packing, correlations between molecular and crystal properties

44) **18.5.1994** Conference on Computational Methods in Chemical Design, Molecular modeling: theory and experiment, Kloster Irsee (Germany)
Empirical intermolecular potentials and crystal structure prediction

45) **24.10.1994** Seminario Nazionale di Chimica Fisica: Chimica fisica del riconoscimento molecolare, Torino (Italy)
Potenziali atomo-atomo nello studio del packing cristallino

46) **2.6.1995** Pfizer Pharmaceutical R&D seminar series, Groton (USA)
Polymorphism in organic crystals: thermodynamic and structural aspects

47) **16.6.1995** Convegno Verso la complessita' molecolare: modelli per la dinamica dei processi reattivi, Monselice (Italy)
Simulazione di solidi cristallini organici: metodi teorici non quantistici

48) **7.8.1995** XVI European Crystallographic Meeting, Lund (Sweden)
Prediction of crystal packing by computer simulation: the static approach

49) **20.9.1995** Seminar Kristallisation fuer die Strukturanalyse und Polymorphie, Gesellschaft Deutscher Chemiker E.V., Bern University (Switzerland)
Crystal packing and polymorphism in molecular solids: database studies and computer simulations

50) **19.10.1995** Italian Pharmaceutical Society, Meeting on solid state pharmaceutics, Milano (Italy)
Computational methods for the characterization of the organic solid state

51) **26.2.1996** Third Italian-Israeli meeting on Chemical Crystallography, Ferrara (Italy)
Computer prediction of organic crystal structures using partial X-ray diffraction data

52) **2.4.1996** British Crystallographic Association Annual Meeting, Cambridge (UK)
Plenary lecture: Are crystal structures predictable?

53) **15.8.1996** XVII Congress of the International Union of Crystallography, Keynote lecture, Seattle (USA)
The crystal packing of organic small molecules

54) **9.9.1996** Scuola dell'Associazione Italiana di Cristallografia, Perugia (Italy)
Relazioni tra struttura e termodinamica

55) **3.4.1997** UCT Research Conferences: Molecular design and synthesis, University of Capetown (South Africa)
Predicting crystal structures

56) **10.6.1997** Dipartimento Chimico Ciamician, Università di Bologna (Italy)
Simulazione al calcolatore di cristalli organici e dei loro precursori allo stato liquido

57) **3.11.1997** NATO ARW Current Challenges on Large Supramolecular Assemblies, Athens (Greece)
Self organization of small organic molecules: crystals, liquids and solutions.
Static and dynamic calculations.

58) **2.12 1997** Polymorphism in Molecular crystals: 100 years of Ostwald's rule. UMIST, Manchester (UK)
Of crystals and other, more heterogeneous things: structure and kinetics of transformation.
What can be done using a computer

59) **18.12.1997** Biochemisches Institut Universitat Zurich
60) **19.12.1997** Laboratorium fur Organische Chemie, ETH, Zurich (Switzerland)
Intermolecular potentials and molecular recognition in crystals, liquids and solutions:
theories and computer simulations.

61) **10.1.1998** NATO ARW Supramolecular engineering of synthetic metallic materials: conductors and magnets, Sitges (Spain
Prediction and control of the organization of organic molecules into crystals: a perspective

62) **21.4.1998** Roche Company, Basel (Switzerland)
Polymorphism in organic crystals: experiments, simulations, predictions

NATO ASI Advances in the computer simulation of liquid crystals, Erice:
63) **11.6.1998** *Intermolecular potentials: Fundamentals*
Fitting intermolecular potentials to empirical models
64) **12.6.1998** *Intermolecular potentials for modeling some simple organic crystals and liquids*

65) **21.8.1998** Academia Leopoldina meeting: Can crystal structures be predicted?, Dresden (Germany)
Molecular crystal structures

66) **23.3.1999** Dipartimento di Matematica, Università di Milano (Italy)
Oggetti simmetrici in chimica e altrove

67) **3.5.1999** Convegno Structural chemistry towards the XXI Century, Weizmann Institute of Science, Rehovot (Israel)
Crystals: How they are made and un-made

68) **16.5.1999** Crystal Engineering, from molecules and crystals to materials, NATO ASI Ettore Majorana Centre, Erice:
Molecular packing in liquids, solutions and crystals: acetic acid as a test case

69) **10.6.1999** The Chemical Society of Denmark Annual Meeting, Odense (Denmark)
Making and un-making crystals in the computer: a probe of the crystallization process

70) **28.4.2000** IBM Research Laboratories, Ruschlikon (Switzerland)
The solid state structure of organic compounds: reality and simulation

71) **1.5.2000** 35th EuChem Conference on Stereochemistry, Burgenstock (Switzerland)
The crystal packing of organic compounds: reality and simulation

72) **8.6.2000** XX Congresso Nazionale della Società Chimica Italiana, Rimini (Italy)
La simulazione dinamica di fasi condensate organiche mediante campi di forza empirici: il futuro della chimica fisica?

73) **27.9.2000** Istituto di Spettroscopia Molecolare CNR, Bologna (Italy)
Chimica teorica per il futuro: simulazione dinamica di fasi condensate organiche

74) **23.11.2000** Dipartimento di Chimica, Università di Ferrara (Italy)
Simulazione dinamica di fasi condensate organiche

75) **3.9.2001** Meeting on Horizons in Hydrogen-bond research, Torino (Italy)
Simulation of hydrogen-bonded organic crystals

76) **20.9.2001** European Federation of Pharmaceutical Societies, Decennial anniversary conference on Rational design of drug materials and drug delivery systems, Strasbourg (France)
Polymorph prediction: myth or reality?

77) **26.5.2002** Annual Meeting of the American Crystallographic Association, keynote lecture, San Antonio, Texas (USA)
Intermolecular interactions at work

78) **27.6.2002** Società Chimica Italiana, Divisioni di Chimica Fisica e Elettrochimica, Ferrara (Italy)
Structure and bonding in organic crystals (Massimo Simonetta memorial lecture)

79) **1.7.2002** CrystEngComm Discussion: Innovation in Crystal engineering, Keynote lecture, The Royal Society of Chemistry, Bristol (UK)
Ten years of experience in polymorph prediction: what next?

80) **10.8.2002** XIX Congress of the International Union of Crystallography, Geneva (Switzerland)
Perspectives in computational molecular dynamics

81) **13.9.2002** Aminoff Symposium, the Royal Academy of Sciences, Stockholm (Sweden)
Understanding crystal nucleation. Can a cheap computer help a million-dollar project?

82) **2.10.2002** Simposio italo francese Crystal Growth: from basic to applied, Accademia Nazionale dei Lincei, Roma (Italy)
The theoretical prediction of crystal structures for organic compounds

83) **10.2.2003** Deutsche Gesellschaft f. Kristallographie, AK14 Workshop, Computational crystallography, Rheinisch-Westfalische Technische Hochschule, Aachen Germany)
Calculation of intermolecular energies from the molecular electron density

84) **25.3.2003** Spring Meeting, Swiss Chemical Society, in Honor of R.Ernst and J.D.Dunitz, ETH Zurich (Switzerland)
Calculation of intermolecular energies from the molecular electron density

85) **26.4.2004** Cutting edge approaches to drug development, Institute of Pharmaceutical Innovation, University of Bradford (UK)
The crystalline state of organic compounds. What a computer can do for you

86) **11.5.2004** Organic Chemistry Seminar, Zurich University (Switzerland)
Intermolecular forces: chemical bonding or chemical bonds?

87) **16.6.2004** Diversity amidst similarity, A multidisciplinary approach to polymorphs, solvates and phase relationships, International School of Crystallography, Erice (Italy)
Computational studies of polymorphs: principles

1-3.9.2004 School of Crystallography, Italian Crystallographic Association, Trieste (Italy)
88) *Dove sono gli atomi? Cristallografia geometrica*
89) *La natura fisica della coesione*

90) **26.9.2004** Pharm. and Thermal Analysis 8 Conference, Ascona (Switzerland)
The lattice energy of organic compounds: thermodynamic facts and computer simulation

91) **12.11.2004** Department of Chemistry and applied biosciences, ETH Zurich, Lugano Campus (Switzerland)
The intermolecular force field of organic compounds: ideas and applications

92) **14.7.2005** in: Ordine e disordine. Il fascino dei cristalli e delle molecole, Giornata in onore di G.Allegra, Politecnico di Milano (Italy)
La previsione delle strutture cristalline: se non ora, quando?

93) **16.9.2005** in: Memorial day: M.Nardelli, Università di Parma (Italy)
Structures and energies: how to spend a lifetime looking at molecules and crystals

94) **16.11.2005** British Crystallographic Association, Chemical Crystallography group autumn meeting: Computational methods applied to crystallography, Daresbury Laboratory (UK)
The calculation of lattice energies of organic crystals: between atom-atom and ab initio

95) **24.2.2006** Incontri Filosofia e Scienza, Comune di Corbetta (Italy)
La chimica: scienza per comprendere il mondo o scienza da sopprimere?

96) **6.7.2006** Giornata Molecole, cristalli e materiali, Università di Alessandria (Italy)
Stereochimica: dalla legge di Bragg a molecole e cristalli in tre dimensioni

97) **Settembre 2006** XXII Congresso della Società Chimica Italiana, Firenze (Italy)
Structural chemistry, past experience and future trends

98) **1.2.2007** Polimorfismo dei Farmaci, Workshop Università di Bologna (Italy)
Sulla definizione di fase cristallina e polimorfismo

99) **9.6.2007** Chemistry Seminar, School of Chemistry, University of Edinburgh (UK)
Intermolecular interaction: from molecules to molecular aggregates

100) **24.7.2007** American Crystallographic Association Annual Meeting, Salt Lake City (USA)
Forty years of struggle with computers over crystallography and intermolecular interactions

101) **24.9.2007** XXXVI Congresso dell'Associazione Italiana di Cristallografia-Meeting Italian Spanish Cryst. Assn, Opening Lecture, Copanello (Italy)
From molecules to crystals: mysteries of aggregation

102) **1.2.2008** Innovation in crystal polymorphism, an International Workshop, University of Bologna (Italy)
Recent computational views on organic polymorphism

103) **31.3.2008** XIII Arden House European conference, The Royal Pharmaceutical Society of Great Britain, London (UK)
Nucleation simulation: what do we know about nucleation at a molecular level?

104) **22.4.2008** Casa della Cultura, Milano (Italy)
Troppa energia dove non serve. La tecnologia produttiva moderna a confronto con l'effetto serra

105) **3.5.2008** European Crystallographic Association, International School on Crystallographic Computing, Gargnano (Italy)
The crystal packing of organic molecules. Intermolecular energies determine crystal symmetry and intermolecular geometry

106) **9.6.2008** ECDM-5, 5th European Charge Density Meeting, Gravedona (Italy)
Charge density and intermolecular potential. Toward a theory of molecular nucleation

107) **24.11.2008** Chemistry Seminar (Department of Pharmacy), University of Innsbruck (Austria)
Polymorphism in organic crystals: facts and fiction

108) **24.4.2009** 27th Annual British Crystallographic Association Spring Meeting, Loughborough:
Thirty years of organic crystal polymorphism in the Cambridge Database

109-110) **May 2009**, Institut Jean Barriol, Facultè de Sciences et techniques –UHP Nancy,
a) Intermolecular interactions. How organic molecules stick together
b) From molecules to crystals: mysteries of aggregation

111) **18-25 April 2010**, International AIC-IUCr School Adsortpion, absoprtion and crystal growth, Gargnano
Molecular simulation of crystal formation

112) **2 september 2010** 5th Bologna Convention on Crystal Forms:
Molecular simulation of crystals by computer: methods and values

113) **6 september 2010** British Association for Crystal Growth Annual Conference, Manchester:
From liquid to crystal. Simulation shortcuts on a long way

114) **15 october 2010**, Department of Organic Chemistry, ETH Zurich:
Reflections on the nature of intermolecular bonding

115) **February 2011**, Department of Chemistry, University of Frankfurt a.M.
Reflections on the nature of intermolecular bonding

116) **4-8 july 2011**, International school Crystallography beyond diffraction, University of Camerino
Modern methods in molecular simulation

117) **11-14 june 2012**, University of Limerick, CGOM2012 International conference:
Modelling pathways for the molecule-to-crystal round trip

118) **Verona 11-14 sept 2012**, 41th Congress of the Italian Crystallographic Association,
Molecular predestination: driving molecules in the twilight zone from liquid to a crystalline state

119) **Bologna, june 2013,** PolyCrystalLine meeting
Structure-activity relationships via molecular simulation. Ionic complexes of organic molecules

120) **Videoconference, oct 27, 2012**: A symposium in Honor of J.McBride, Yale University,
Modelling pathways from molecule to crystal

121) **November 21-22, 2013, Politecnico di Milano**: Meeting 'Natta's seeds grow'
Natta's seeds with genetic modification. Crystallography at the University of Milano

122) **March 21, 2014, ETH-Zurich, Chemistry seminars**
God's hand:racemic vs. chiral synthesis and crystallization

123) **May 28, 2014, ETH Lugano branch, CECAM Workshop**:
Molecular simulations of crystallization from solution

124) **August 27, 2014, Universitè de Lausanne, CECAM Workshop** 'Addressing challenges for first-principles based modeling of molecular materials':
From liquid to solid by biased Monte Carlo simulation

125) **July 1, 2015, Symposium for the 50th anniversary of the Cambridge Structural Database, Cambridge University and CCDC:**
Twenty-five years of CSD mining: chemical bonds and chemical bonding

126) **September 14, 2015, Congresso annuale dell'Associazione Italiana di Cristallografia,**
Vercelli (for the award of the Mammi Medal) :
Things done and things yet (not) to be done: crystallography at large, 2015-2030

127) **September 7-11, 2016 Rimini, AIC International Crystallography School 2016:**
Polymorphism, stability and phase transitions in crystals: theory, experiments and applications
Opening Lecture: From atoms to crystals: how, when and why
The intermolecular potential: nature and applications
Molecular simulation of crystals: methods and results