



Aldo Gamba

 UNIVERSITY OF INSUBRIA



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Contact data

Full Professor

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Biography

University of Milano: 1962 -1975; 1992 -1980 - 1961 degree in Industrial Chemistry; 1962 -1965: Associate Professor in Chemical Physics; 1971-1975: Assistant in Chemical Physics; 1964-1975: charged with the courses of Chemical Physics Laboratory, Theoretical Chemistry, Molecular Spectroscopy; 1985-1989: Teacher in the Specialistic School in Biotechnology, 1984-1989 Member of the Council of Department of Physical Chemistry;

University of Sassari: 1975-1982: Full professor in Chemical Physics, 1975-1982: Director of the Institute of Chemical Physics; President of the Chemistry Degree Council; Director of the Scientific Computational Centre; 1976-1982: Dean of the Faculty of Science; ; 1982-1990 – Member of CUN Committee for chemical research funds; 1983-1989: Full Professor at the University of Milano; 1983-1987: Member of the managing board of Italian Association of Chemical Physics; 1992: Lecturer in the Doctorship of Chemical Physic in the Swiss University of Geneva, Lousanne and Friburg;; 1998-2000: member of administration council of Villa Erba spa (Como).

Qualifications and awards

1969: Free Docent in Theoretical Chemistry; 2001-2003: member of the national board of Italian Association of Zeolites; 2004-2006: President of Italian Association of Zeolites (Onlus);

Research interests

Starting from 1962 the research interests developed as follows: 1962-1970, studies on models based on empirical techniques to investigated structure and reactivity and spectroscopic properties of organic molecules; 1970-1980: theoretical studies on organic paramagnetic systems, investigated experimentally by EPR and ENDOR spectroscopies made in the laboratories built up in Milano and Sassari; 1980-to day: studies of time evolution of systems of chemical relevance by simulation techniques to obtain a complete picture of non-reactive and reactive processes. In particular, first principle molecular dynamics, the Car Parrinello method was widely explored and employed to investigate microporous materials.

Teaching experience and appointments

Professor of physical chemistry and lecturer in different years in chemical kinetics and molecular dynamics, molecular spectroscopy, environmental chemical physics, chemical physics for cultural heritage.

Representative publications

1994-1996: president of CCL of Chemistry
Co-ordinator of XV and XVI cycle of PHD in Chemical Science
2001-2004 and 2004-2007: Dean of the Faculty of Science in Como
From 2004, member of "Atheneum Resource Commission".

E. Fois, A. Gamba, G. Tabacchi, First Principles Simulation of the Intracage Oxidation of Nitrite to Nitrate Sodalite, *Chem., Phys.*, 2000, 329, 1

A. Pelenschikov, G. Morosi, A. Gamba, S. Coluccia, G. Martra, L.G.M. Petterson, "Can the Three-Coordinated Mg Site of MgO Accomodate More than One CO Molecule?" *J. Phys. Chem B*, 2000, 104, 11497-11500.

E. Fois, A. Gamba, E. Spanó, "Electronic Properties of new zeolitic supralattices" *Phys. Chem, Chem. Phys* 2001, 3, 1877-1882.

E. Fois, A. Gamba, G. Tabacchi, S. Quartieri, G. Vezzalini, "On the collective properties of water molecules in one dimensional zeolitic channels", *Phys. Chem. Chem. Phys.* (2001).

E. Fois, A. Gamba, G. Tabacchi, "Water Molecules in single File: First-Principles Studies of One Dimensional Water Chains in Zeolites", *J. Phys. Chem B*, 2001, 105, 3012-3016

E. Fois, A. Gamba, E. Spanó, G. Tabacchi, "Ab initio Simulation of Zeolites of Technological Interest Including Heteroatoms in the Framework" *Proc. of 7 European Conference on advanced Materials and Processes*, 2001, Rimini (Italy), 137-138.

M. Cavalleri, A. Pelenschikov, G. Morosi, A. Gamba, S. Coluccia, G. Martra, "Dissociative Adsorption on defect sites of MgO: a combined IR Spectroscopic and Quantum Chemical Study" *Studies in Surface Science and Catalysis*, 140, 131-139, A. Gamba, C. Colella, s. Coluccia Eds, 2001, Elsevier Science B.V.

E. Fois, a. Gamba, G. Tabacchi, "Intracage Chemistry: Nitrite to Nitrate oxidation via molecular oxygen." *Studies in Surface Science and Catalysis*, 140, 251-268, A. Gamba, C. Colella, s. Coluccia Eds, 2001, Elsevier Science B.V.

E. Fois, A. Gamba, A. Tilocca, "Structure and dynamics of the flexible triple helix of water inside VPI-5 molecular sieves", *J Phys. Chem. B.*, 2002, 106, 4806-4812.

O. Ferro, S. Quartieri, G. Vezzalini, E Fois, A. Gamba, G. Tabacchi; "High pressure behaviour of bikitaite: an integrated theoretical and experimental approach", *Am. Min.*, 87, 1415-1425, 2002.

A. Alberti, E. Fois, A. Gamba, "A Molecular Dynamics study of the behaviour of sodium in low albite", *Amer. Miner.*, 88, 1-10, 2003.
Fois, A. Gamba, A. Tilocca, M.A. Vanoni, " First-Principle Molecular Dynamics investigation of the D-aminoacid oxidative reaction catalyzed by flavoenzymes", *Biochem.*, 2002, 41, 14111-

14121.

C.Ceriani, E.Fois, A.Gamba, "The Role of extra framework cations on the structure of dehydrated Li- ABW. A computer simulation study." *Micro.Meso Materials*, 2002,57,73-81.

E.Fois, A.Gamba, E.Spanó "Ab Initio investigation of a Ti center in Offretite", *Studies in Surface Science and Catalysis*, 142 , Tech Reports, Elsevier, Amsterdam,2002.

E.Fois, A.Gamba, G.Tabacchi, O.Ferro, S.Quartieri, G.Vezzalini, A theoretical investigation on pressure –induced changes in the vibrational spectrum of zeolite Bikitaite, *Studies in Surface Science Catalysis* , 142, pg.1877-1884,2002.

E.Fois, A.Gamba, A.Tilocca, "On the unusual stability of Maya Blue paint: Molecular Dynamics simulations" *Micro. Meso. Mat.* , 2003, 57, 263-272

E. Fois, A. Gamba, E. Spanó, G. Tabacchi, "Rotation of molecules and ions in confined Spaces first-principles simulation study" *J. Mol. Struct.*, 2003, 644, 55-66

E.Fois, A.Gamba, G.Tabacchi, S.Coluccia, G.Martra, "Ab Inizio Study of Defect Sites in Surfaces of Mesoporous Silica" *J. Phys. Chem..B*, ottobre 2003 , *J.Phys.Chem.*,107 (39): 10767-10772 (2003)

E.Fois, A. Gamba, G. Tabacchi, S. Coluccia, M. Martra, " Properties of defect centres on nanothick Silica layers: an ab initio investigation". *J. Porous Mat*, 2003 in corso di stampa.

O.Ferro, S.Quartieri, G.Vezzalini, C.Ceriani, E.Fois, A.Gamba, G.Cruciali "Dehydration dynamics of bikitaite:Part I. In situ synchrotron powder X-ray diffraction study".*Am. Miner.*,2004,89,94-101.

E. Fois, A. Gamba, E. Spanó, "Competition between Water and Hydrogen Peroxide at Ti Centre in Titanium Zeolites. An Ab Initio Study.", *J. Phys Chem. B.*, 108 (28): 9557-9560 (2004).

C.Ceriani, A. Laio, E. Fois, A. Gamba, R. Martonak and M. Parrinello. "Molecular dynamics simulation of reconstructive phase transitions on anhydrous Li-ABW zeolite" *Physical Rew. B* 70, 113403 (2004).

Ceriani C., Fois E., Gamba A., Tabacchi G., Ferro O., Quartieri S., Vezzalini G. "Dehydration dynamics of bikitaite: PartII. Ab initio molecular dynamics study" *American Mineralogist*, 89 (1): 102-109 Jan 2004

Fois E., Gamba A., Spano E. "Ab inizio molecular dynamics simulation of the interaction between water and Ti in zeolitic systems" *Journal of Physical Chemistry B*, 108(1): 154-159 Jan 8 2004

E.Fois, A.Gamba, G.Tabacchi, R. Arletti, S.Quartieri, G.Vezzalini, "The "template" effect of the extra-framework content on zeolite

compression: The case of yugawaralite", Amer. Mineral., 90,28-35 (2005).

E. Fois, A.Gamba, G.Tabacchi "Electronic Spectra of Ti (IV) in Zeolites: An Ab Initio Approach", ChemPhysChem 2005, 6, 1237-1239

Oxide Based Materials - New sources, novel phases, new applications

E.Fois, G.Gamba, G.Tabacchi, S.Quartieri, R.Arletti, and G.Vezzalini
"High-pressure behaviour of yugawaralite at different water content: an ab initio study" ChimPhysChem, 2005, 271-280

Oxide Based Materials - New sources, novel phases, new applications

R.Tubino, E.Fois, A.Gamba, G.Macchi, F.Meinardi, and A.Minoia

"Conjugated molecules in nanochannels: nanoengineering for optoelectronics" ChemPhysChem 2005, 501-510

Ettore Fois, Aldo Gamba, Cinzia Medici, and Gloria Tabacchi
"Intermolecular Electronic Excitation Transfer in Confined Space: A First-Principles Study" ChemPhysChem 2005,6, 1-7