UNIVERSITÀ DEGLI STUDI DI MILANO

Angelo Sironi
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- 1972: Degree in Chemistry (cum laude) at the University of Milan.
- 1972-1982: Research Assistant at the Laboratory of structural chemistry of the University of Milan;
- 1982-1983: SERC Post Doctoral Fellowship at North London Polytechnic working with Prof. M. McPartlin (London) and Prof. J. Lewis (Cambridge);
- 1983-2000: Associated professor of General Chemistry;
- 2000-Present: Full Professor of General Chemistry at the Milan University;
- Member of INSTM (Interuniversity Consortium of "Materials Science and Technology);

SCIENTIFIC FIELDS OF INTEREST

Prof. Angelo Sironi, one of the pioneers of *ab-initio* powder diffraction as a tool for determining the structure of phases failing to afford suitable single crystals, works in the field of Structural Chemistry. His expertise concern both the *experimental* determination of crystal structures and the *theoretical* interpretation of structural information. In particular he has studied the nature of metal-involving interactions in organometallic and coordination compounds using diffraction, molecular mechanic, quantum chemistry (EHT, DFT and ab-initio methods) and Bader's "quantum theory of atoms in molecules". As a member of Paolo Chini enterprise, the once famous "Milano clusters school", he has a longstanding experience in the field of metal carbonyl clusters. Presently, he is interested in organic-inorganic hybrid materials with particular emphasis on the determination of three-dimensional models of new functional materials for optics and optoelectronics, and thermally robust coordination polymers, capable of molecular recognition.
Author of more than three hundred publications on high impact journals, his expertise is well represented by the following activities:

- Determination of the molecular and crystal structure of organometallic compounds by single crystal diffraction.
- Determination of the molecular and crystal structure of crystallographically simple systems by *ab-initio* X-ray (and Neutron) powder diffraction.
- Experimental determination of the accurate electron densities of crystals from X-ray (and Neutron) diffraction at low temperature (20-120K). Use of *Ab-intio* computations on molecules and extended arrays for the rationalization of the experimental accurate electron densities according to Bader's quantum theory of atoms in molecules.
- High pressure single crystal crystallography.
- Use of Density functional theory for understanding the origin of conformational preferences and the solution dynamics of organometallic molecules.
- Molecular Mechanics computations within the crystal lattice.
- Use of complementary information derived from DSC, TGA, SEM, AFM, IR microscope, hot stage microscopy.

Some recent publications are:

1. X-Ray Powder Diffraction Characterizaton of Polymeric Metal Diazolates.
   N. Masciocchi, S. Galli, A. Sironi,
   Techniques in Inorganic Chemistry, **2010**, 15-52, CRC Press.

2. The α and β forms of oxalic acid di-hydrate at high pressure: a theoretical simulation and a neutron diffraction study
   Piero Macchi, Nicola Casati, William G. Marshall and Angelo Sironi
   CrystEngComm., **2010**, *12*, 2596 - 2603.

3. High pressure modification of organic NLO materials: large conformational re-arrangement of 4-aminobenzophenone
   Elena Marelli, Nicola Casati, Fabia Gozzo, Piero Macchi, Petra Simoncic and Angelo Sironi
   CrystEngComm., **2011**, *13*, 6845 - 6849.

4. The role of molecular packing on the absorption properties of the two polymorphs of $[Re_2Cl_2(CO)_6$4,5-(Me_3Si)2pyridazine]
   Silvia Tavazzi, Leonardo Silvestri, Peter Spearman, Alessandro Borghesi, Pierluigi Mercandelli, Monica Panigati, Giuseppe D'Alfonso, Angelo Sironi, Luisa De Cola
   Cryst. Growth & Desing, **2012**, *12*, 742-749.

5. Synthesis, Reactivity, Electrochemical Behavior, and Crystal Structure of a Family of Multivalent Metal Carbido−Carbonyl Clusters Based on the Rh10(C)2Au4−6 Framework
   Laura Cherchi, Alessandro Fumagalli, Serena Fedi, Piero Zanello, Fabrizia Fabrizi De Biani, Franco Laschi, Luigi Garlaschelli, Piero Macchi, and Angelo Sironi
   Inorg.Chem., **2012**, 51, 9171-9180.

6. Probing Hydrogen Bond Networks in Half-Sandwich Ru(II) Building Blocks by a Combined ^{1}H DQ CRAMPS Solid-State NMR, XRPD, and DFT Approach
   Michele R. Chierotti, Roberto Gobetto, Carlo Nervi, Alessia Bacchi, Paolo Pelagatti, Valentina Colombo, Angelo Sironi
   Inorg.Chem., **2014**, 53, 139-146.

7. On the self-condensation of aminoguanidine leading to 1,1,4,10,10-pentaamino-2,3,5,6,8,9-hexaazadeca-1,3,5,7,9-pentaene (structure elucidation through X-ray powder diffraction)
   Bruno Tasso, Gerolamo Pirisino, Federica Novelli, Davide Garzon, Roberta Fruttero, Fabio Sparatore, Valentina Colombo, Angelo Sironi
   Tetrahedron, **2014**, 70, 8056-8061.

8. Tetrameric Silver(I) Complex with Bridging N-Heterocyclic Carbene Ligands: $[(iPrIm)Ag(NO_3)]_4$.
   Della Pergola, R.; Bruschi, M.; Sironi, A.; Colombo, V.; Sironi, A.
   Organometallics **2014**, 33, 5610–5613.

9. An Interacting Quantum Atoms Analysis of the Metal–Metal Bond in $[M_2(CO)_8]^n$ Systems
   Davide Tiana, E. Francisco, P. Macchi, Angelo Sironi and A. Martin Pendàs
   J. Phys. Chem. A, **2015**, *119*, 2153-2160.