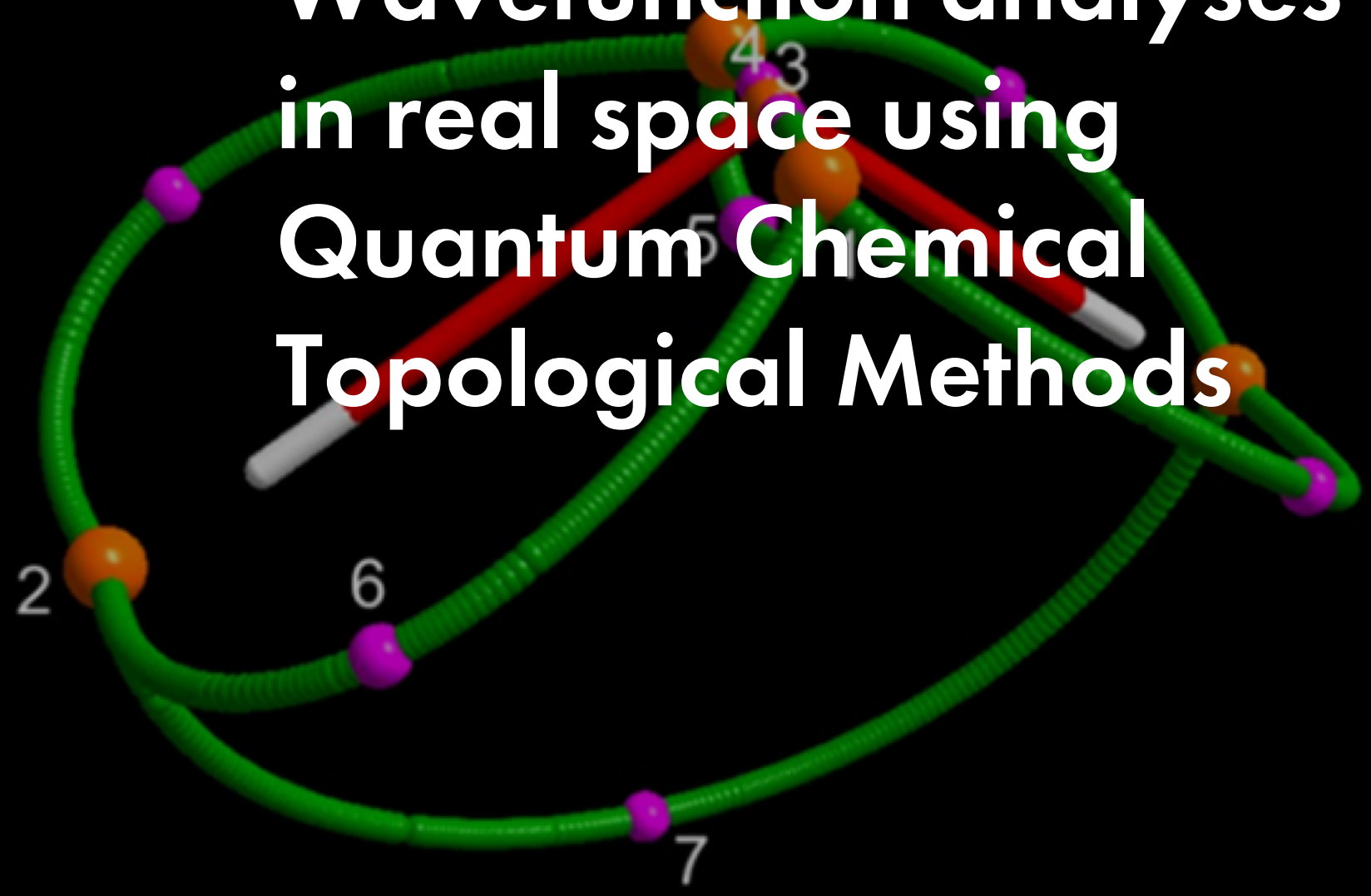
Seminar
May 20
17:00

Online

# Wavefunction analyses in real space using Quantum Chemical Topological Methods




## Carlo Gatti

Research Director at CNR-SCITEC
(Istituto di Scienze e Tecnologie Chimiche,
"Giulio Natta", Milano)

## Speaker introduction

Carlo Gatti got the Doctor degree in Chemistry and Theoretical Physical Chemistry in 1978 from the Università degli Studi di Milano (UNIMI), Italy. He has been visiting scientist or professor in many international labs, including: Mc Master University, Hamilton, Canada (Prof. RFW Bader's); SUNY Buffalo, USA (Prof. P. Coppens, in 1999 and 2000); LCM3B, Universitè de Nancy, France (Prof. C. Lecomte, in 2007); RWTH Aachen, Dept. of Physics, Germany (Prof. M. Wüttig, 2017-2018), etc. Since 2010 he is one of the six international partners of the Center for Materials Crystallography, a Centre of Excellence based on funding from the Danish National Research Foundation.

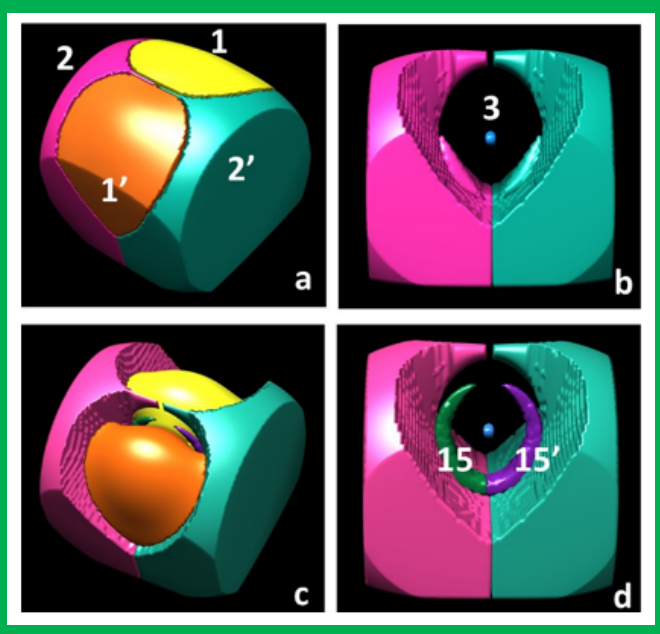
Gatti's scientific expertise includes:

- Quantum Chemical Topology (QCT) methods and Software development (TOPOND-98, TOPXD, XD, NCI-Milano, topological code TOPOND in CRYSTAL-14 and CRYSTAL-17) for QCT methods implementation to molecular and condensed phase systems and to ab-initio and X-ray derived electron densities
- Development of new chemical bonding descriptors in real space, like the Source Function, SF
- Application of QCT methods to exotic bonding in systems under pressure
- Applications of QCT methods to material science (in particular thermoelectric materials, phase change materials, Li and Na batteries, etc.);
- Extension of Non-Covalent Interactions Reduced Density Gradient approach to X-ray derived experimental electronic densities in crystals
- Development of QCT methods for spin polarized systems
- Application of QCT methods in HPLC enantiomers separation, by extending the SF to the Electrostatic Potential
- Modern revisit of the Pauling's Bond Valence Models

Gatti has been awarded the prestigious Gregori Aminoff Prize 2013 from the Royal Swedish Academy of Sciences, along with Prof. Mark Spackman. "for developing experimental and theoretical methods to study electron density in crystals, and using them to determine molecular and crystalline properties. Gatti has written 129 peer-reviewed papers (>9100 citations, h-index=51) and 14 book chapters, most of them on charge density analysis and QCT issues. Along with Piero Macchi, he edited the 2012 Springer book on Modern Charge Density Analysis (>34k downloads thus far).

## Seminar abstract

Thoughtful searches for more and more performing materials or of materials with novel properties and functions require a profound understanding of their structure-property relationships. While the detailed knowledge of the structure of a material, either through experimental and/or in silico approaches, is a necessary and fundamental prerequisite for its study, it should not be overlooked that the geometrical, electronic (and magnetic) structure of a material are ultimately related to its chemical bonding features. And as an obvious consequence, material's properties are in turn determined by these same features.
The present lecture will give a broad overview of the most widely adopted chemical bonding investigation tools within the realm of the so called Quantum Chemical Topology (QCT) methods. For each of them some representative applications will be carefully discussed. Rather than offering a comprehensive list of literature examples, the main focus of the lecture will be on highlighting the basic theory behind the presented methods, along with a discussion of their physical roots and limits, so as to eventually favor their proper and hopefully profitable use.

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