Thursday, Feb 22, at 16:00-17:00

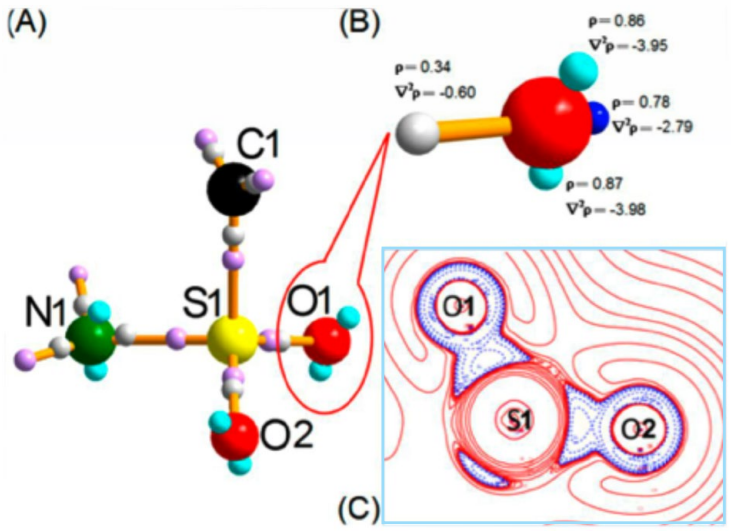
Skoltech, Blue Bldg, room 407

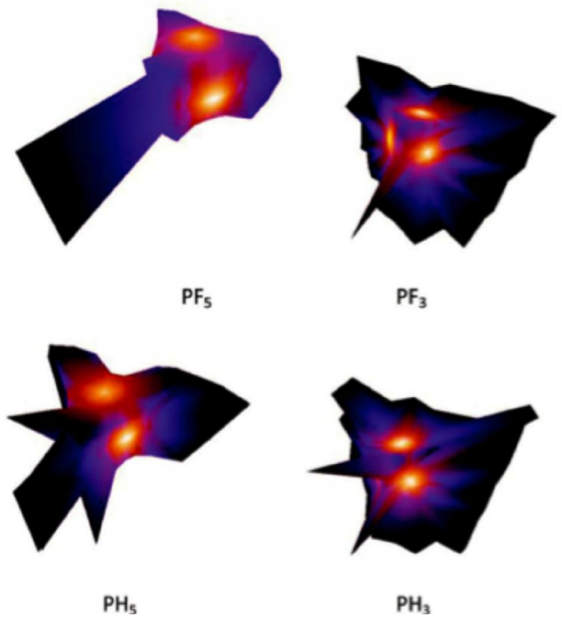
Skoltech

Skolkovo Institute of Science and Technology

Development of new methods

into the framework of Bader's Theory and their application





Speaker

Christian Tantardini
Novosibirsk State University

Abstract:

The chemical behavior of atoms and molecules is entirely defined by the distribution of their electron density. It is by studying the electron density that key concepts of chemical importance come about, such as chemical bonding, reactivity, atomic hybridisation, and the existence of electric multipole moments. The last decades have seen the development of modern theories to study charge density and the most influential to date has been the quantum theory of atoms in molecules (QTAIM), developed by R.W. Bader and colleagues in the 1980s. At the heart of QTAIM there exists the central concept of atomic basins, which subdivide a molecule into regions that encase an atomic nucleus: an atom. With the success of Bader's original theory a series of different topological tools were developed as source function (SF) (eq.1), delocalization indexes, Espinosa indexes, domain-averaged Fermi hole analysis and so on. A novel approach for SF was developed through its calculation from electron densities generated by plane wave (PW) methods. To show the validity of developed method on a series of test systems the results obtained at PW level were compared with those previously obtained through AE methods. Furthermore, a new topological tool is developed, the Bader energy density, PBADER (eq.2), which is introduced and applied to the study case of chemical reactivity a priori **of PH_5.**

$$SF(r,\Omega) = -\frac{1}{4\pi}\int_{\Omega} d\mathbf{r}' \frac{\nabla^2\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \quad (1)$$

$$P_{BADER}(\Omega) = \frac{E(\Omega)}{V(\Omega)} \quad (2)$$

Biography:

Christian Tantardini received in 2012 Bachelor's Degree in Chemistry and Industrial Chemistry at the University of Study of INSUBRIA, Como (Italy) and he was graduated with 110/110 in only 2 years with the thesis title: "Tunnel Effect in Carbon Nanotubes - Simplified Models" under supervision of Dr. Massimo Mella. He continued his study obtaining in 2014 the Master of Science in Chemistry at the University of Milano, Milano (Italy) and he was graduated with 110/110 and praise with the thesis title: "Development of novel topological tools for the real space investigation of spin density in organometallic complexes" under supervision of Dr. Leonardo Lo Presti and Dr. Carlo Gatti. In the last 3 years at the Novosibirsk State university under supervision of Prof. Elena V. Boldyreva his research has included the development of new methods in quantum chemistry and a study of a range of organic and inorganic systems using quantum chemical and topological approaches in both gas and solid phase systems.

Looking forward to seeing you!