Physics Colloquium

Michigan Technological University

Thursday, November 11, 2010 at 4:00 pm

Room 139 Fisher Hall

Theoretical Investigation of Metal-Organic Frameworks

Loredana Valenzano

Department of Physics

Michigan Technological University

Abstracts: In recent years, metal organic frameworks (MOFs) gained great interest because of their promising properties for gas storage, gas purification, catalysis, and molecular recognition. A wide range of specific applications can emerge from them involving energy processes, molecule capture, drug delivery and sensing. MOFs are crystalline porous materials formed by metal-oxide clusters connected three-dimensionally by polyfunctional organic ligands that act as spacers, creating 3D open porous structures, characterized by very high pore volume and surface area. Their peculiar structure, that shows big permanent porosity, results in the capability of hosting molecules, from hydrogen to carbon dioxide, to organic species. Moreover, the choice of appropriate metals and organic linkers (and their functionalization) potentially implies the possibility to design and explore big families of these new materials.

In this colloquium, the characterization and the prediction of structural, electronic, vibrational and adsorption properties of different MOFs species will be described as obtained with an periodic *ab-initio* approach. The aim is to show how nowadays it is possible to confirm and predict, quantum mechanically, properties of such complex materials. Also, accurate *ab-initio* results can serve as strategic link between experiments and large scale computational simulations (and vice versa) in a synergic investigation process of isolating *well behaving* new species.

Bio: After receiving her Master degree in Particle Physics at the University of Turin (I), Loredana moved to Southampton (UK) where in 2003 she got her PhD in Theoretical Physical Chemistry. For the successive two years, she worked as a postdoc at the University of Leiden (NL). In 2005, she moved back to her hometown in Italy, where for more than five years she was a postdoc in the theoretical chemistry group of the University of Turin, where she studied properties and behaviour of crystalline solids. In the last two years, she mainly worked on the *ab initio* characterization of properties of metal-organic frameworks (MOFs) through international academic and industrial collaborations (Norway, Germany, Spain). Among other scientific initiatives, in May 2010, she organized in Lausanne (CH) the international workshop “Gas Separation and Gas Storage Using Porous Materials”. In summer 2010, she moved to Houghton to work as Assistant Research Scientist and Instructor at MTU, where she is involved in the computational studies of energetic materials and silicon nanowires.

MichiganTech