NUS National University of Singapore | Department of Mechanical Engineering
Faculty of Engineering

You are cordially invited to our:
Department Seminar

Topic: **Virtual Instruments for Spectroscopy: Development, Validation and Applications in Life- and Material- Sciences**

Speaker: **Prof. Vincenzo Barone**
Scuola Normale Superiore, Pisa, Italy

Date: **2 October 2013, Wednesday**

Time: **12.00pm to 1.00pm**

Venue: **E1-06-04** *(map of NUS can be found at http://map.nus.edu.sg/*

Host: **Dr. Sergei Manzhos**

Abstract

The increased necessity to design new responsive materials with unique properties, which could be tuned and controlled by means of appropriate external sources, for specific applications in different sectors such as aerospace, electronics, ceramics, packaging, drug delivering and targeting, requires a cooperative experimental/computational effort. Interpretation and prediction of the spectroscopic properties of these composite systems have been obtained through calibrated computational protocols defined in our group. In the framework of the ERC Advanced Grant Project DREAMS "Development of a Research Environment for Advanced Modeling of Soft Matter", GA N° 320951 we are extending our new multifrequency virtual spectrometer [1] toward larger systems including nanoparticles and polymers. In this way, molecular motions and supra-molecular interactions in real-size structures can be captured combining all levels of theory, ranging from classical molecular dynamics simulations (CMDs) to full quantum mechanics calculations (QMc). The combination of CMDs, based on accurately parameterized force fields, and QMc, based on density functional theory (DFT) and its time-dependent extension (TD-DFT) have been used to simulate both the absorption and emission spectra of dyes in solution [2] and interacting with different kinds of nanoparticles [3], and succeeded in elucidating the mechanisms which determined the modifications of different spectroscopic properties (IR, Raman, UV-vis, etc.) observed experimentally. The photophysical properties of organic chromophores incorporated (grafte/dispersed) in apolar polymer matrices have also been studied in detail [4] and the influence of the polymer bundle on the dynamics and conformational properties of the dopants together with the configurations responsible for both the absorption and emission spectra have been identified.

[1] V. Barone, A. Baiardi, M. Biczisko, J. Bloino, C. Cappelli, F. Lipparini, Implementation and validation of a multi-purpose virtual spectrometer for large systems in complex environments, PHYSICAL CHEMISTRY CHEMICAL PHYSICS 14, 12404-12422 (2012).
[2] F. Lipparini, F. Egidi, C. Cappelli, V. Barone, The Optical Rotation of Methyloxirane in Aqueous Solution: A Never Ending Story?, JOURNAL OF CHEMICAL THEORY AND COMPUTATION 9, 1880-1884 (2013).
[3] A. Pedone, J. Bloino, V. Barone, Role of host-guest interactions in tuning the optical properties of coumarin derivatives incorporated in MCM-41: a TD-DFT investigation, JOURNAL OF PHYSICAL CHEMISTRY C 116, 17807-17818 (2012).
[4] G. Prampolini, F. Bellina, M. Biczysko, C. Cappelli, L. Carta, M. Lessi, A. Pucci, G. Ruggeri, V. Barone, Computational design, synthesis, and mechanocromic properties of new thiophene-based π-conjugated chromophores, CHEMISTRY 19, 1996-2004 (2013).

About the Speaker

Vincenzo Barone is a full Professor of Theoretical and Computational Chemistry at the Scuola Normale Superiore in Pisa, Italy President of the Italian Chemical Society for the period 2011-2014, fellow of the International Academy of Quantum Molecular Sciences (IAQMS), and of the Accademia dei Lincei. He is author of more than 600 papers mainly devoted to the development, validation and application of new computational strategies for the study of stereo-electronic, dynamical, and environmental effects on physical-chemical properties of molecules and supramolecules. His most important theoretical contributions concern the development of new density functionals, solvent models and effective treatments of harmonic and anharmonic effects on spectroscopic properties. His works have received more than 30000 citations (3520 in 2012) with an h-index of 72.

Admission is free. All are welcome to attend.