AVVISO DI CONFERENZA

Il giorno **VENERDI' 20 GENNAIO 2012,**
alle ore **15**, nell'**AULA A1 (III piano)**
del DIPARTIMENTO DI SCIENZE CHIMICHE
E FARMACEUTICHE,
Università di Trieste, Edificio C11, Via Giorgieri 1

il Prof. ANTONINO POLIMENO

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dell'Università degli Studi di Padova

terrà una conferenza dal titolo:

Computational approaches to modeling of ESR and NMR observables

Tutti gli interessati sono cordialmente invitati

Il Direttore del Dipartimento di Scienze Chimiche e Farmaceutiche

Prof. Paolo Tecilla

Computational approaches to modeling of ESR and NMR observables

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Understanding the dynamic behavior of molecules is of fundamental importance to describe their chemical functions and reactivity. A wealth of information on molecular relaxation processes can be extracted from magnetic resonance spectroscopic data, but additional theoretical and computational insight is required. In particular, cw-ESR and NMR relaxation data can be interpreted by a basic theoretical approach defined within the Stochastic Liouville Equation (SLE) formalism, i.e. the direct inclusion of motional dynamics in the form of stochastic (Fokker-Planck / diffusive) operators in the super Hamiltonian governing the time evolution of the system.[1] Modeling based on the SLE approach requires the characterization of magnetic parameters (e.g. hyperfine and Zeeman tensors) and the calculation of ESR observables in terms of spectral densities. The magnetic observables can be pursued by the employment of Density Functional Theory (DFT) which are adapted, provided that hybrid functionals are employed, to the accurate computation of structural properties of molecular systems.[2] In this presentation I shall discuss the. 1) determination of geometric and local magnetic parameters by quantum-mechanical DFT calculations taking into account solvent and, when needed, vibrational averaging contributions; 2) numerical solution of a stochastic Liouville equation in the presence of diffusive rotational dynamics, based on 3) parameterization of diffusion rotational tensor provided by a hydrodynamic model. cw-ESR spectra are simulated with minimal or no resorting to fitting procedures, proving that the combination of sensitive ESR spectroscopy and sophisticated modeling can be highly helpful in providing 3D-structural and dynamic information on molecular systems in complex environments.

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3. V. Barone and A. Polimeno, Phys. Chem. Chem. Phys. 8, 4609 (2006); A. Polimeno, M. Zerbetto, L. Franco, M. Maggini, C. Corvaja, J. Am. Chem. Soc. 128, 4734 (2006)