RICHIESTA SEMINARIO DI DIPARTIMENTO

Giovedì 16 Marzo Ore 15:00, Aula V Edificio Caglioti (NEC)

Titolo: Ground- and excited-state properties in theoretical quantum chemistry: stochastic models and approximations from atoms to biochromophores.

Relatore: Dr. Emanuele Coccia (CNR Institute of Nanoscience, Modena, Italy)

Proponente: Prof. Enrico Bodo

Quantum Monte Carlo (QMC) methods [1] are becoming a powerful and reliable alternative to wave-function methods (post Hartree-Fock approaches) and density-functional theory (DFT) for quantum chemical calculations, thanks to their favorable scaling with the system size and to the extremely good suitability to high performance computing infrastructures, such as petascale architectures. In this seminar, recent methodological developments and applications to problems of physical and chemical interest are presented, based on the use of variatonal and diffusion Monte Carlo (VMC and DMC, respectively) techniques. First, the thermodynamics of the water-splitting reaction is computationally investigated by means of a model cobalt complex that catalyzes the overall reaction; VMC and DMC are seen to overperform accurate quantum-chemistry approaches, as coupled cluster [2]. Second, the combination of high-level VMC and many body Green's function theory calculations allows us to define an accurate theoretical protocol for the study of the absorption spectra of biochromophores, as the retinal protonated Schiff base [3,4] and the anionic forms of oxyluciferin [5], even in the presence of the protein environment treated at classical level of theory [3,4]. Finally, the direct extension of QMC to the computation of excited-state properties is explored by defining the linear-response theory in the VMC framework [6]; a collection of VMC results for the low-lying excitations of the beryllium atom is compared with reference values, showing a satisfactory agreement.

[1] B. M. Austin, D. Y. Zubarev and W. A. Lester, Jr., *Chem. Rev.* **112**, 263 (2012)

[2] S. Chu, E. Coccia, M. Barborini and L. Guidoni, *J. Chem. Theory Comput.* **12***,* 5803 (2016)

[3] E. Coccia, D. Varsano and L. Guidoni, *J. Chem. Theory Comput.* **9***,* 8 (2013)

[4] D. Varsano, E. Coccia, O. Pulci, A. Mosca Conte and L. Guidoni, *Comp. Theor. Chem.* **1040-1041,** 338 (2014)

[5] E. Coccia, D. Varsano and L. Guidoni, *J. Chem. Theory Comput.,* submitted

[6] E. Coccia, B. Mussard, R. Assaraf, C. Umrigar and J. Toulouse, *Adv. Quantum Chem.*, submitted

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