UNIVERSITÀ DEGLI STUDI DI MILANO

SEMINARI ERC

ERC GRANT
SEMICOMPLEX

Data ***Lunedì 28 Novembre 2016, ore 14:30***
Aula Bianchi, Dipartimento di Chimica

Oratore **Dr. Jaime Suarez, Universidad Autonoma de Madrid**

Titolo**:** **GridTDSE: Cartesian coordinate-based wave packet propagations in QMD**

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Quantum Molecular Dynamics (QMD) simulations provide accurate pictures of what happens in the molecule during a certain process. The evolution of the nuclear structure is ruled by the Time Dependent Schrödinger Equation (TDSE), involving both vibrational and rotational motions. The choice of the adequate coordinate system is then a crucial stage. Standard curvilinear coordinates usually involve complex quantum Hamiltonians that must be approximated in high-dimensional systems (N>3 dimensions). In contrast, the Cartesian-coordinate approach yields the exact form of the ro-vibrational Dynamics, and the extrapolation to larger systems is straightforward. The GridTDSE method is presented here is an appealing computational tool that solves the TDSE in Cartesian coordinates through a parallelization strategy, fulfilling the requirement of high-demanding memory calculations. The application of GridTDSE to several systems of varying nature, both bounding and dissociating, will be showed.