UNIVERSITÀ DEGLI STUDI DI MILANO

DIPARTIMENTO DI CHIMICA

Data ***Martedì 22 Gennaio 2019, ore 15:30***
Aula G15, Settore Didattico Golgi

Oratore **Prof. Dmitrii V. Shalashilin**, School of Chemistry, University of Leeds, Leeds LSE 9JT, UK; *d.shalashilin@leeds.ac.uk*

Titolo **Trajectory guided basis sets of Coherent States for quantum dynamics.**

Coordinatore **Michele Ceotto,** *Dipartimento di Chimica*

Brief review of quantum molecular dynamics methods, which use trajectory guided basis sets of Coherent States[1, 2], will be presented. The methods are capable of treating quantum systems with many degrees of freedom and their applications range from nuclear wave packets describing nonadiabatic photochemical reactions to electron dynamics in strong laser field. In particular the details and new applications of Multiconfigurational Ehrenfest (MCE) approach will be presented[3, 4] as well as several versions of recently developed *Ab initio* Multiple Cloning (AIMC) first principle direct dynamics[5, 6]. Its features, such as sampling techniques and interpolations for matrix elements will be described, as well as recent AIMC application to ultrafast nonadiabatic photodynamics[7] and nonadiabatic energy transfer in conjugated molecules[8]. MCE method has also been applied to simulation of the ultrafast X-ray diffraction experiments[9].

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