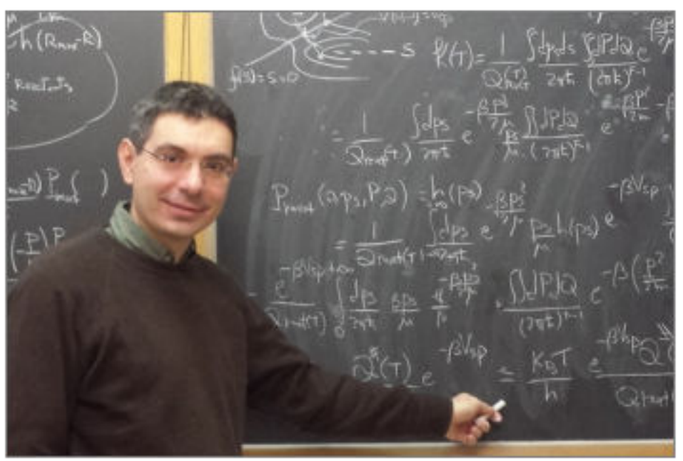
Seminar Michele Ceotto



Prof. Michele Ceotto, Università degli Studi di Milano, will be visiting our group from Wednesday 13th To Thursday 14th of February. He will hold a seminar on Wednesday 13th, h. 15.30, Aula 20 with the following title: Semiclassical Molecular Dynamics and its Implementation for Spectroscopic Calculations of High Dimensional and Condensed Phase Molecular Systems.

Abstract: I will present some novel semiclassical methods designed for spectroscopic calculations of high dimensional and/or condensed phase systems. Some of the methods are based on a “divide-and- conquer” approach, where the full dimensional spectra are obtained as a composition of several lower dimensional ones. Others exploit hierarchically the different levels of accuracy of different semiclassical propagators. All methods are within 10-20 wavenumbers Mean Absolute Error average respect to the exact or experiments when available, and are amenable to ab initio molecular dynamics simulations.