UNIMORE Dipartimento di Scienze Fisiche, Informatiche e Matematiche

UNIVERSITÀ DEGLI STUDI DI MODENA E REGGIO EMILIA

CNRNANO MODENA S3

FIM-S3 SEMINAR

Ab initio calculation of energy relaxation rates in dense plasmas and liquid metals

Friday May 31th, 2024 – 11.00 (sharp)

S3 Seminar Room, 3rd Floor, Physics building
Remote link: Teams

Speaker

Jacopo SIMONI – University of Wisconsin-Madison, USA

Abstract

The study of the interaction between electrons and ions in solids under a variety of conditions is of fundamental importance in condensed matter physics. Despite the small electron to ion mass ratio these interactions are never fully adiabatic due, in the case of metallic systems, to the continuum of electronic states available at the Fermi level allowing for a coupling with the ionic degrees of freedom. The non-adiabatic transitions result in exchanges of small amounts of energy that maintain thermal equilibrium between electrons and ions, and drive the irreversible evolution towards thermal equilibrium from a non-equilibrium state.
In solid metals, the non-adiabatic interactions are described in terms of electron-phonon interactions. In liquid metals or warm dense systems where the electron-phonon picture no longer holds because ions have the ability to travel throughout the system, the basic properties of these interactions remain largely unexplored.
In this work I have systematically explored, for the first time, these non adiabatic properties in the case of a wide variety of systems under different conditions and temperatures and pressures. Clearly, a detailed description of non adiabatic couplings with first-principles simulations re- mains a formidable challenge. However, a simplified coarse-grained description avoiding an explicit account of all the electronic degrees of freedom is possible.

Host: Marco Govoni

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