



Università degli Studi di Roma "Tor Vergata"
Dipartimento di Fisica

SEMINARIO TEORICO

Prof. Giancarlo Rossi

(University of Rome "Tor Vergata")

“A (little) progress in Density Functional Theory”

Abstract

We give a novel and simple proof of the Density Functional Theory expression for the interatomic forces that drive the motion of the atoms in ab initio Molecular Dynamics, alternative to the one ensuing from the Hellmann-Feynman theorem. The proof is based on the observation that the ground state electronic energy, seen as a functional of the external potential, is the Legendre transform of the Hohenberg-Kohn functional, which is in turn a functional of the electronic density. In this way we demonstrate that there is no room for the so-called Pulay force corrections and we provide a rigorous foundation to the Potential Functional Theory

Mercoledì

11 Ottobre 2017

ore 14,30

Aula Seminari “U.M.Grassano”