NANO COLLOQUIA 2025 - S3 SEMINAR

## *Functional theory of the occupied spectral density*

## Thursday April 10, 2025 – 14:30

ON-SITE - S3 Seminar Room, Third Floor, Physics Building
ONLINE  - https://tinyurl.com/NanoColloquia

## Speaker: Andrea Ferretti - Cnr Nano

**Abstract**
We address the problem of interacting electrons in an external potential by introducing the occupied spectral density as a fundamental variable. First we formulate the problem using an embedding framework [1] and prove a one-to-one correspondence between a spectral density and the local, dynamical external potential that embeds it into an open quantum system. Then, we use the Klein functional to (i) define a universal functional of the spectral density, (ii) introduce a variational principle for the total energy, and (iii) formulate a non-interacting mapping suitable for numerical applications. The resulting equations, which involve local and dynamical potentials, are then solved by using the algorithmic inversion method [2, 3, 1] based on a sum-over-poles to represent propagators.
At variance with time-dependent density-functional theory, this formulation aims at studying charged excitations and electronic spectra with a functional theory, although an explicit and formally correct description of all electronic levels could also lead more naturally to accurate approximations for the total energy.

[1] A. Ferretti, T. Chiarotti, N. Marzari, Phys. Rev. B 110, 045149 (2024)
[2] T. Chiarotti, N. Marzari, A. Ferretti, Phys. Rev. Research 6, L032023 (2024).
[3] T. Chiarotti, A. Ferretti, N. Marzari, Phys. Rev. Research 4, 013242 (2022).

**Host:** Massimo Rontani (segreteria.s3@nano.cnr.it)

DRIVING THE EXASCALE TRANSITION

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