NANO COLLOQUIA 2024 - S3 SEMINAR

Accurate treatment of metallic screening in Many-Body calculations from first principle

Thursday March 14, 2024 – 14:30
ON-SITE - S3 Seminar Room, Third Floor, Physics Building
ONLINE - https://tinyurl.com/NanoColloquia

Speaker Giacomo Sesti - Cnr Nano S3 and Unimore

Abstract

Many-Body Perturbation Theory calculations within the GW approximation have proven to be a reliable scheme for the computation of quasiparticle (QP) band structures of materials. While QP corrections in metallic systems are generally smaller than in semiconductors, they are crucial for accurate spectroscopic descriptions, especially in low-dimensional systems.
The computational cost of GW poses however challenges, particularly in accurately describing the screened potential in both frequency and k-space for metals. One of the challenges is the inclusion of the long-wavelength limit of intraband transitions, usually treated by adding a Drude term at the plasmon energy. However, the ab-initio determination of the plasmon energy is generally demanding. In addition, the Drude method may be too simplistic for certain metals and semimetals, since more than one pole may be needed in the description of interband transitions[1].
In this colloquium, I discuss a recently developed method for performing efficient QP computations in metals. This approach, initially developed for 2D semiconductors, involves Monte Carlo integration and interpolation techniques[2,3], leading to significant speed-ups in k-point convergence[4]. Extending its applicability to 3D and 2D metals, I demonstrate the accurate evaluation of the screened potential, allowing for efficient QP computations without additional parameters. The method reproduces QP band structures with reduced k-point grids, offering a streamlined approach for studying metallic systems.

1) D. A. Leon, C. Cardoso, T. Chiarotti, D. Varsano, E. Molinari, and A. Ferretti. Phys. Rev. B, 104, 115157 (2021).
2) F. H. da Jornada, D. Y. Qiu, and S. G. Louie, Phys. Rev. B 95, 035109 (2017).
3) W. Xia , W. Gao, G. Lopez-Candales, Y. Wu, W. Ren, W. Zhang and P. Zhang npj Comput. Mater. 6, 118 (2020).
4) A. Guandalini, P. D'Amico, A. Ferrett, D. and Varsano. npj Computational Materials 9, 44 (2023).

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