Superconducting DFT in the SIESTA method and code

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Superconductivity is an intrinsically quantum phenomenon, defying the classical picture of dissipative current flow. It is one of the striking cases where quantum effects manifest at the macroscopic scale. Conventional superconductivity is predicted by the Bardeen, Cooper, and Schrieffer (BCS) theory. Unconventional superconductivity, instead, is described by the Bogoliubov-de Gennes (BdG) theory, a generalization of BCS to model inhomogenous superconductors. However, to predict complex phenomena such as topological superconductivity, it is necessary to model *on the same footing* atomistic and superconducting properties.

In this talk, we present SIESTA-BdG: the implementation of Superconducting Density Functional Theory (SCDFT [1]) in SIESTA [2, 3], a first-principles method and code for materials simulation which uses pseudopotentials and a localized basis set. SCDFT combines the BdG and Density Functional Theory (DFT) frameworks in a unified approach to describe both conventional and unconventional superconductivity. We demonstrate the validity, accuracy, and efficiency of our implementation by predicting physically relevant quantities (superconducting charge density, band structure, superconducting gap features, density of states) for conventional (Pb, Nb) and unconventional (FeSe) superconductors. We use SIESTA-BdG to demonstrate proximity induced superconductivity in normal/superconductor heterostructures (PbTe/Pb). The semi-phenomenological approach of SIESTA-BdG can further be used to model topological superconductivity and forms the basis for modelling quantum transport in the superconducting state.

References

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[3] A. García et al., J. Chem. Phys. **152** (2020) 204108
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Figures

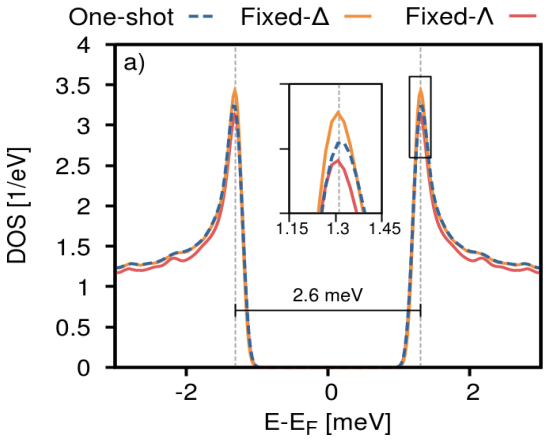

Figure 1: Density of States of bulk Pb in the superconducting phase computed with SIESTA-BdG, Comparison among three different self-consistent field schemes (one-shot, fixed pairing potential Δ, fixed superconducting coupling strength Λ) to converge the normal and anomalous densities. Figure from Ref. [4].