# Ab-initio simulations of transition metal-superconductor interfaces

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The realisation of Majorana-based topologically protected qubits requires a careful design and optimization of material interfaces for superconductor (SC) / topological insulator (TI) heterostructures. To this end, we perform ab-initio simulations to investigate the superconducting properties at the interface of transition-metal overlayers (M = Os, Ir, Pt, Au) deposited on a Nb(110) film. Our density functional theory simulations are based on the full-potential Korringa-Kohn-Rostoker (KKR) Green function method and its Kohn-Sham Bogoliubov-de Gennes (KS-BdG) extension [1, 2]. In our study, we explore the possibility of controlling the work function mismatch through the overlayer, which is essential to overcome the band bending effect impeding the superconducting proximity at typical SC/TI interfaces. Furthermore, we uncover the proximity induced superconductivity in the metal overlayers and discuss related details in their electronic structure. Our findings show that some of these structures might be promising material candidates for interfacing a TI with a superconductor without unwanted band bending effects at SC/M/TI interfaces.

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