

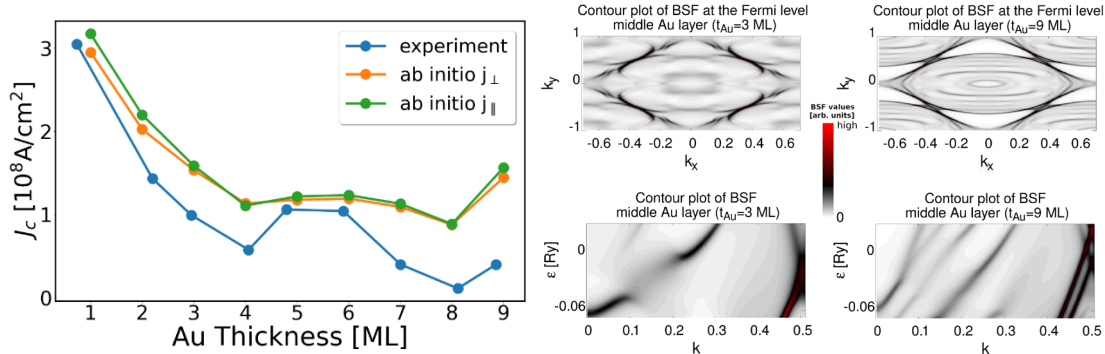
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### **Ab initio Theory of Quantum Size Effects in Josephson Junctions**

In this work, we develop a fully microscopic theoretical description of superconducting transport through quantum-confined metallic spacers and demonstrate its predictive power by direct comparison with experiments on epitaxial Nb/Au/Nb Josephson junctions. Our results show that electronic structure effects alone can control Andreev transport in clean, nonmagnetic heterostructures. The study focuses on Nb(110)/Au(111)/Nb(110) trilayers with monolayer-level control of the Au spacer thickness. Experiments reveal pronounced nonmonotonic variations of the critical current density, superconducting coherence length, and transition temperature as functions of the Au thickness. To explain these observations, we formulate a fully relativistic Kohn--Sham--Dirac--Bogoliubov--de~Gennes theory and implement it within a layered Green-function Korringa--Kohn--Rostoker framework.

This *ab initio* approach treats superconductivity, spin--orbit coupling, and the realistic multi-orbital band structure on equal footing. Unlike quasi-classical models, it explicitly captures quantum confinement and interface-induced hybridization at the atomic scale. Our calculations show that confinement in the Au spacer gives rise to thickness-dependent quantum well states whose crossings at the Fermi level strongly modify the low-energy quasiparticle spectrum responsible for Andreev reflection. As it is demonstrated on Figure 1, the theory quantitatively reproduces the experimentally observed oscillations of the Josephson critical current and at the same time identifies their microscopic origin. In particular, we find that changes in the Au electronic structure drive a crossover from ballistic to tunneling transport without invoking disorder, magnetism, or phenomenological parameters. For larger Au thicknesses, our calculations predict the emergence of additional Andreev bound states associated with quantum well subbands near the Brillouin-zone edge. These states induce a spatially nonuniform proximity-induced superconducting order parameter in the Au layer, corresponding to Cooper pairing with finite center-of-mass momentum. This unconventional superconducting state appears in zero magnetic field and enhances both the critical current and the transition temperature.

By providing a quantitative, parameter-free description of proximity-induced superconductivity at the atomic scale, this work establishes first-principles theory as a powerful design tool for superconducting heterostructures. The results demonstrate that quantum size effects enable systematic control of Josephson transport through band-structure engineering, highlighting the central role of *ab initio* theory developed at Quantum Materials Research group of the Wigner RCP.



**Figure 1.** The relationship of the normal state electronic structure to the critical current (a) Parallel and perpendicular to the plane critical current as a function of the Au's thickness at  $T=6 \text{ K}$  compared to experimental results. (b),(c) Fermi surface of the middle Au monolayer for 3 ML and 9 ML Au thickness, respectively. (d),(e) Contour plot of Bloch spectral function (BSF) along the high-symmetry line  $k_x=2k_y$  ( $k$  is measured in  $\pi/a$  units) for 3 and 9 ML Au thickness, respectively.

### References:

- [1] Yamazaki, H. ; Csire, G. ; Kucska, N. ; Shannon, N. ; Gyorffy, B. ; Takagi, H. ; Újfalussy, B., *Quantum Size Effects on Andreev Transport in Nb/Au/Nb Josephson Junctions: A Combined Ab Initio and Experimental Study*, Physical Review Letters 134, 196002 (2025) <https://www.webofscience.com/wos/woscc/full-record/001494090900004>