Modelling emergent effects in low coordination geometries during metallic nanojunction formation

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Quantum phenomena that are not observed in bulk metals, but which manifest in low coordination geometries such as few-atom contacts [1, 2], suspended monatomic wires [3, 4] and free surfaces [5-7] are modelled by means of a combination of classical and quantum mechanical atomistic simulations; including, classical molecular dynamics, tight binding models and density functional theory. The roles played by the parent crystal structure and local electronic structure of the metal atoms in these low coordination environments are explored. Since emergent quantum properties, such as enhanced magnetism along suspended monoatomic wires [4], also directly affect the local geometry and electronic structure of the nanocontacts, a more accurate theoretical description is needed to resolve discrepancies between existing theoretical results and experiment. Additionally, such a description should lead to more informed predictions about metallic nanocontacts created from body-centered metal samples, which have not been the object of many studies thus far. In this work, we study the formation and rupture of gold, copper and tungsten nanocontacts, with the view of extracting trends that can be extrapolated to other transition metals, which are also frequently employed in the experiments, including platinum, iron, and silver.

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