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Transport in Molecular Junctions with Different Metallic Contacts JOHN LAWSON, CHARLES BAUSCHLICHER, NASA Ames Research Center — Ab initio calculations of phenyl dithiol connected to Au, Ag, Pd, and Pt electrodes are performed using non-equilibrium Green's functions and density functional theory. For each metal, the properties of the molecular junction are considered both in equilibrium and under bias. In particular, we consider in detail charge transfer, changes in the electrostatic potential, and their subsequent effects on the IV curves through the junctions. Gold is typically used in molecular junctions because it forms strong chemical bonds with sulfur. We find however that Pt and Pd make better electrical contacts than Au. The zero-bias conductance is found to be greatest for Pt, followed by Pd, Au, and then Ag. (Physical Review B, 74, (2006), p 125401)

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