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A theoretical investigation of the porphyrin-gold junction: applications to molecular wires. MATT MCKENZIE, ZORABEL LEJEUNE, JAYNE GARNO, BIN CHEN, Louisiana State University — An important step in the miniaturization of electronic devices involves molecular wires and junctions at the nanoscale level. Porphyrins are a promising material for such objects because of their unique electronic, chemical, and optical properties. The model porphyrin used in this study is a free based tetra-substituted with two phenyl rings and two pyridyl rings as peripheral groups which could provide a mechanism for enhanced electron transfer. The goal of this study is to elucidate the electron transfer paths between the model porphyrins and Au(111). The orbital structures and properties are determined using Car-Parrinello molecular dynamics. The geometry of the porphyrin on the gold surface is explored; from a complete reorientation of the molecule with respect to the surface to different orientations of the pyridyl groups. The calculated electronic conductivity, using the Kubo-Greenwood formula, will be compared to experimental findings using conductive probe Atomic Force Microscopy.

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