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Orbital resolved electron transport in single molecule contacts KRISTIAN THYGESEN, ROBERT STADLER, MIKKEL STRANGE, KARSTEN JACOBSEN, Center for Atomic-scale Materials Physics, Technical University of Denmark — We have performed a theoretical study of the phase-coherent electron transport in three different molecular junctions consisting of hydrogen, CO and bi-pyridine connected to Pt and Au leads. In all three cases we find good agreement with experimental results. We use a Green's function transport scheme in combination with density functional theory and a Wannier function basis set. The transport characteristics of the three molecules differ substantially ranging from complete transparency in the case of hydrogen to resonant tunneling through the LUMO state of the bi-pyridine molecule. By reconstructing the molecular orbitals of the contacted molecule and subsequently calculating the transmission with different orbitals removed from the basis set, we can directly test the individual contributions to the transmission from each molecular orbital and thereby obtain a detailed picture of the conduction mechanism.

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