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Exploring the lead dependence of single-molecule conductance from first principles: The case of H_2 molecular junctions K.H. KHOO, Dept of Physics, UC Berkeley, J.B. NEATON, The Molecular Foundry, LBNL, STEVEN G. LOUIE, Dept of Physics, UC Berkeley, The Molecular Foundry, LBNL
— Although the transport properties of several single-molecule junctions have now been reported, only a few studies have systematically examined the sensitivity of the junction conductance to the choice of metallic contacts. Recent break-junction experiments have revealed significantly lower conductance for H_2 molecular junctions when Pt leads were replaced with Pd,[1,2] suggesting a dramatic difference in electronic coupling between the molecule and lead. In this work, we examine this coupling directly by computing the conductance of H_2 with several different metallic contacts using an *ab-initio* scattering state approach[3] based on density functional theory.We find that by substituting Pt with Pd leads, the low-bias electron transport crosses over from a ballistic to an off-resonance tunneling regime, leading to a conductance smaller than unity in agreement with experiments. The extent to which substituting different leads may be used to tune the transport properties of this and other simple single-molecule junctions will be discussed. This work was supported by the NSF Grant No. DMR04-39768 and U.S. DOE Contract No. DE-AC03-76SF00098. [1] R. H. M. Smit *et al.*, Nature (London) **419**, 906 (2002). [2] Sz. Csonka *et al.*, Phys. Rev. Lett. **93**, 016802 (2004). [3] H.J. Choi, M.L. Cohen and Steven G. Louie, to be published.

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