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**Theoretical study of the conductance through hydrogen decorated Pd nanojunctions** K.H. KHOO, UC Berkeley and LBNL, J.B. NEATON, The Molecular Foundry, LBNL, STEVEN G. LOUIE, UC Berkeley and LBNL — In a recent experiment, the conductance through Pt and Pd nanocontacts have been measured in an $H_2$ atmosphere.[1] This work suggested that electron transport is mediated by individual $H_2$ molecules, which are reported to have nearly perfect conductance, i.e., with a value of a single quantum unit conductance. However, subsequent measurements on Pd nanocontacts in $H_2$ yielded data with a half of a quantum unit of conductance, and this new result was attributed to hydrogen being dissolved in the Pd contacts.[2] In this study, we have computed the conductance of atomic and molecular hydrogen between Pd and $PdH_x$ nanocontacts using an *ab-initio* scattering-state approach[3] based on density functional theory and with a local-orbital basis set. Our results show that the conductance is highly sensitive to both the junction geometry and the hydrogen content of the lead. We find that significant hybridization reduces the conductance significantly below that of one quantum unit. The implications of our results for the interpretation of experiments are discussed.This work was supported by NSF Grant No. DMR04-39768 and by DOE under Contract No. DE-AC03-76SF00098. Computational resources have been provided by NERSC and NPACI. [1] R.H.M. Smit *et al.*, Nature **419**, 906 (2002). [2] Sz. Csonka *et al.*, Phys. Rev. Lett. **93**, 016802 (2004). [3] H.J. Choi, M.L. Cohen, Steven G. Louie, to be published.

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