First-principles study of the conductance of hydrogen-decorated nanojunctions

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In a recent experiment, the conductance through Pt and Pd nanocontacts have been measured in an H_2 atmosphere.[1] The measurements 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 $2e^2/h$. However, subsequent measurements with Pd nanocontacts in H_2 yielded only half the conductance, a result attributed to hydrogen being dissolved in the Pd contacts.[2] In this study, we have computed the conductance of molecular hydrogen between Pt, Pd, and PdH 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 the presence of hydrogen, the junction geometry, and the lead chemistry. In particular, the computed conductance across the hydrogen molecule differs appreciably for Pt, Pd and PdH leads; for Pt leads, we obtain a conductance close to one quantum unit, while calculations with Pd and PdH leads result in a conductance significantly less than unity. Implications for the interpretation of recent 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 **416**, 906 (2002).

[2] Sz. Csonka *et al.*, Phys. Rev. Lett. **93**, 016802 (2004).

[3] H. J. Choi, M. L. Cohen, and S. G. Louie, to be published.