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**NEGF Transport Simulation on Pd<sub>4</sub>-cluster Functionalized CNTs**

CHAO CAO, Quantum Theory Project and Department of Physics, University of Florida, ALEXANDER KEMPER, Quantum Theory Project and Department of Physics, YAO HE, Quantum Theory Project, University of Florida, HAI-PING CHENG, Quantum Theory Project and Department of Physics, University of Florida — We have investigated the conductance response of the Pd-cluster functionalized CNTs to hydrogen environment using DFT+NEGF method. Experiments find that the semiconducting CNTs behave very differently from metallic CNTs, and suggest that the semi-conducting ones are good candidates for hydrogen sensors. By comparing the simulation results for the (5,5) metallic and the (8,0) semiconducting CNTs, we are able to reveal the underlying physics behind this phenomena. This work is supported by the DOE grant number DE-FG02-02ER45995. The authors want to thank NERSC, CNMS/ORNL and the University of Florida High Performance Computing Center for providing computational resources and support that have contributed to the research results reported within this paper.

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