

Abstract Submitted  
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**First-Principle Calculation on Hydrogen Dissociation on Pd-doped CNT**<sup>1</sup> CHAO CAO, ALEXANDRE KEMPER, YAO HE, HAI-PING CHENG, QTP, Univ. of Florida — We have calculated hydrogen dissociation on Pd-doped (5,5) CNT using density functional theory (DFT), and examined its influence on the conductance of CNT using a non-equilibrium green's function (NEGF) method. Our results show that the hydrogen dissociation is barrier-less on edge of Pd cluster, while on the top of Pd cluster the molecule would not automatically dissociate. Calculations also show that a dense doping with Pd cluster would modify the band structure of CNT substantially such that the doped tube becomes a semi-metal. The dissociation of hydrogen molecule will further change it into a semiconductor. Our NEGF calculations confirmed the band structure calculation, and suggested that Pd-doped CNT could be used as a hydrogen sensor device by measuring the conductance change of the device induced by hydrogen dissociation.

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