ATOMIC, ELECTRONIC, AND TRANSPORT PROPERTIES OF SEMICONDUCTING AND MOLECULAR NANOWIRES AND THEIR CONTACTS

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Nanowires have been a subject of continuing research efforts due to fundamental interest in their properties, as well as because of their potential technological applications. In this talk we discuss theoretical investigations, using first-principles quantum mechanical methods, pertaining to two classes of nanowires: (1) semiconductor nanowires with metal contacts, and (2) molecular nanowires supported by, or embedded in, metal electrodes.

(1) We review our previous investigations of hydrogen-passivated silicon nanowires supported by aluminum contacts [1], and describe our recent studies of CdSe nanowires passivated by phospho-organic molecules of varying chain length, with gold contacts attached at the ends. In both cases we find formation of Schottky barriers similar to those of extended systems, and development of interfacial dipoles well localized at the interface [1, 2]. Chain length effects of the passivating molecules are discussed.

(2) Spin-density-functional calculations of tip-suspended gold chains, with molecular oxygen, or dissociated oxygen atoms, incorporated in them, reveal structural transitions for varying lengths [3]. The nanowires exhibit enhanced strength for both oxygen incorporation modes, and upon stretching, tip atoms join the wire. With incorporated molecular oxygen the wire conductance is about $1(2e^2/h)$, transforming to an insulating state beyond a critical length. Our results are used to interpret recent experiments on oxygen contating Au nanowires [4]. The nanowire conductance with embedded oxygen atoms is low, $0.2\ (2e^2/h)$, and it develops magnetic moments localized on the oxygens and the neighboring Au atoms.

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