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First-principles study of bio-conjugated ultra-thin silicon nanowires: Interaction with a PNA-RNA double helix XIAOLIANG ZHONG, WILLIAM SLOUGH, RAVINDRA PANDEY, CRAIG FRIEDRICH, Michigan Technological University — We present the results of a first-principles study based on density functional theory of peptide nucleic acid (PNA) - ribonucleic acid (RNA) double helix conjugated silicon nanowires (SiNWs). The effects of a hexane linker functionalization, probe PNA strand immobilization, and target RNA strand hybridization on the electronic states of the ultra-thin SiNWs in a dry condition are investigated. All of these effects appear to marginally modify the core silicon states of the nanowires, manifested by a low level of p-doping in SiNWs. The intrinsic energy gap of the SiNWs is essentially unchanged, though there exist mid-gap states contributed by the PNA/RNA molecules which tend to localize near the Fermi energy. Overall, the bio-conjugation considered does not appear to significantly affect the intrinsic electronic and transmission states of the ultra-thin SiNWs.

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