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**Schottky Barrier Heights in CNT-Metal Junctions from First-principles** NICHOLAS SINGH-MILLER, NICOLA MARZARI, Massachusetts Institute of Technology — Fundamental understanding of the electronic properties at the junction between a carbon nanotube (CNT) and a substrate is important for the practical application of CNT-based devices. Here, we use density functional theory (DFT) to probe the properties of the CNT-metal interface, paying particular attention to the Schottky barrier heights (SBH). We focus on the junction between a semiconducting (8,0)CNT and aluminum or palladium, chosen as paradigmatic examples of a simple metal and a transition metal, respectively. We obtain SBHs from the potential lineup, examining the effects of geometry at the interface and the functionalization of the CNT on the SBH.

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