First-principles studies on the metal contact with carbon-based nanomaterials

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For the experimental realization of the device using carbon-based nanomaterials (CNMs), such as graphene (GR) or carbon nanotubes(CNTs), it is important to understand the properties of the interfaces with metal electrodes. Even there have been extensive studies on the metal-GR (or CNT) interfaces with various metal elements, there are some missing metal elements, such as indium. In this paper, we present the first-principles calculations based on density functional theory on the metal-GR (or CNT) interfaces, including indium and other metal elements. We will discuss the metal-CNMs interface properties with respect to the chemical properties of metal elements, themselves.