Supporting Information

Contact Resistance Properties between Nanotubes and Various Metals from Quantum Mechanics

Yuki Matsuda, Wei-Qiao Deng, and William A. Goddard III*

Materials and Process Simulation Center (MC74-139), California Institute of Technology, California 91125, USA

Figure S1. Optimized geometries of the top (top) views and side views (bottom) of (a) Ti, (b) Pd, (c) Pt, (d) Cu, and (e) Au deposited on a graphene 4 x 4 sheet. (Unit cell for optimization is graphene 2 x 2 sheet which is fixed at 4.89×4.89 Å). (gray graphite, green metal first layer, orange metal second layer, light blue metal third layer)