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Coupling of carbon nanotubes and graphene nanoribbons by the titanium and vanadium nanowires: First-principles study[1] CHI-HSUAN LEE, CHIH-KAI YANG, Graduate Institute of Applied Physics, National Chengchi University — We investigate the combined structure of a carbon nanotube (CNT) and graphene nanoribbon (GNR) through the adsorption of a titanium or vanadium nanowire (NW), using first-principles calculations. The binding energy depends upon the stacked configuration and is much larger than that between the two subsystems without the nanowire. The band structure reveals strong hybridization between d orbitals of the transition metal and p orbitals of the carbon atoms. Furthermore, if the CNT is deposited near the border of GNR, structural stability is enhanced and magnetic moments of the edge atoms are reduced. The result points to possible application for synthesizing nanowires in nanoelectronic devices.

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