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Electronic transport properties of sawtooth penta-graphene nanoribbons under edge passivation by non-metallic atoms

The transport properties of sawtooth penta-graphene nanoribbons (SS-PGNRs) are investigated using density functional theory in combination with nonequilibrium Green function. The configurations are theoretically studied in terms of a bare edge and edges terminated by non-metallic atoms (H, P, Si) such as : symmetrical edge terminations (HH-SS-PGNR, PP-SS-PGNR and SiSi-SS-PGNR) and alternate edge terminations (PH-SS-PGNR and SiH-SS-PGNR). It is found that SS-PGNR band gap can be controlled through changing various edge termination, which leads to the transition from a semiconductor to a half-metal or to a metal. In effect on transport properties, P and Si atoms improve significantly the current intensity in alternate cases. The obvious reduction of current is observed in HH-SS-PGNR and PP-SS-PGNR. Interestingly, oscillation current-voltage characteristic appears when PGNR is passivated symmetrically by Si atoms. These outcomes derive from the strong dependence of SS-PGNRs on type of terminated atom at the edge of ribbon and could be used to design novel nano-electronic devices.

Authors: Mr TRUNG PHUC, Vo (Can Tho University); Dr BICH THAO, Pham Thi (Can Tho University); Prof. THANH TIEN, Nguyen (Can Tho University)

Presenter: Mr TRUNG PHUC, Vo (Can Tho University)