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Electronic and transport features of sawtooth penta-graphene nanoribbons via substitutional doping

In this work, electronic and transport properties of a pristine sawtooth penta-graphene nanoribbon (SSPGNR) and sawtooth penta-graphene nanoribbons doping with Silic, Nitrogen, Phosphor (Si-SSPGNR, N-SSPGNR, P-SSPGNR) are studied systematically by density-functional theory in combination with the non-equilibrium Green's function formalism. Pristine sample and three doped samples in a similar position are terminated with H atoms. To explore in detaided the electronic and electron transport features, we compute and discuss about the structure properties, bandstructure, density of states, I-V curve, device density of states and tranmission spectrum. Our result shows that doping affects dramatically on the electronic nature and the I-V characteristic of samples. More specifically, the intensity of current of N-SSPGNR and P-SSPGNR increase by 8 orders of magnitude compared to SSPGNR while the one of N-SSPGNR change negligible. However, there are also considerable differences in I-V curves of samples doping with N and P. Our findings indicate that the doping by N, P can effectively modulate the electronic and transport properties of SSPGNRs which has not been studied so far.

Authors: Mr VO TRUNG, Phuc (Can Tho University); Dr PHAM THI BICH, Thao (Can Tho University); Prof. NGUYEN THANH, Tien (Can Tho university)

Presenter: Prof. NGUYEN THANH, Tien (Can Tho university)