Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information

Site-dependent stability and electronic structure of single vacancy point defects in hexagonal graphene nano-flakes

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Ionization Potential

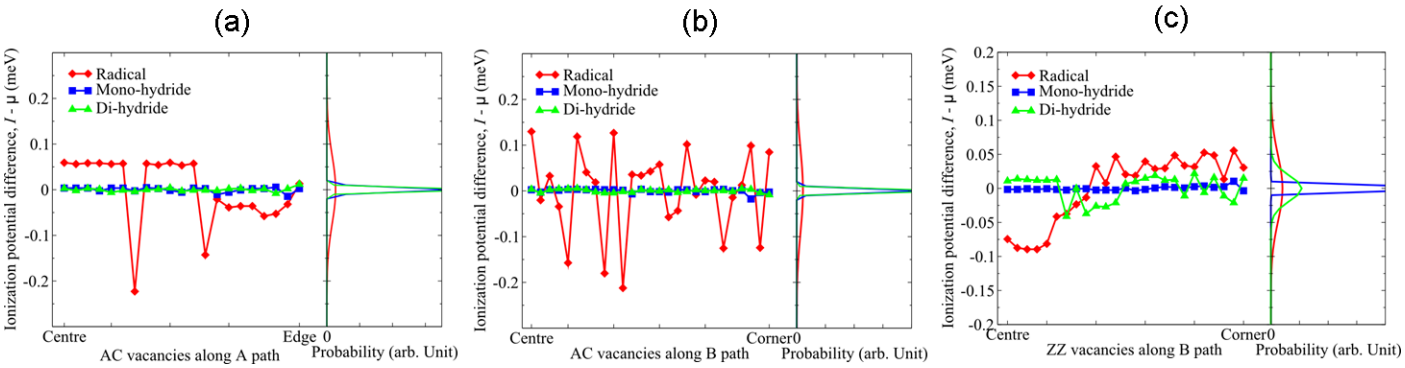

Figure S1. The ionization potential, respect to the average value in various sets, is given for (a) all the vacancy structures along the path A in AC-edged radical, mono-hydride, and di-hydride terminated hexagonal graphene nano-flakes, (b) all the vacancy structures along the path B in AC-edged radical, mono-hydride, and di-hydride terminated hexagonal graphene nano-flakes, and (c) all the vacancy structures along the path B in ZZ-edged radical, mono-hydride, and di-hydride terminated hexagonal graphene nano-flakes.

Electron Affinity

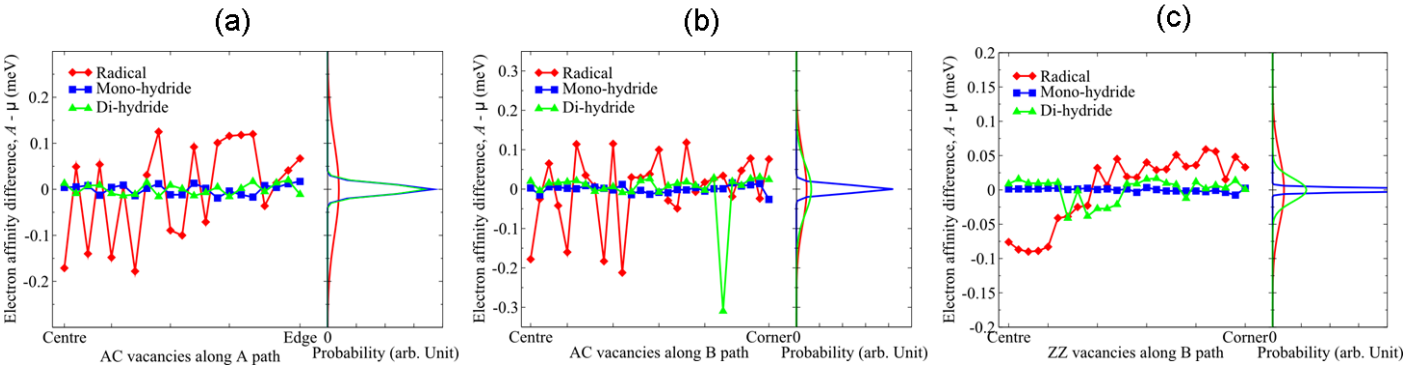

Figure S2. The electron affinity, respect to the average value in various sets, is given for (a) all the vacancy structures along the path A in AC-edged radical, mono-hydride, and di-hydride terminated hexagonal graphene nano-flakes, (b) all the vacancy structures along the path B in AC-edged radical, mono-hydride, and di-hydride terminated hexagonal graphene nano-flakes, and (c) all the vacancy structures along the path B in ZZ-edged radical, mono-hydride, and di-hydride terminated hexagonal graphene nano-flakes.