Supplementary: NJC

Metal cluster-deposited graphene as adsorptive materials for *m*-xylene

Anchalee Junkaew,[a] Chompoonut Rungnim,[a] Manaschai Kunaseth,[a] Raymundo Arróyave,[b] Vinich Promarak,[c] Nawee Kungwan,[d] and Supawadee Namuangruk [a,*]

[a] *NANOTEC, National Science and Technology Development Agency (NSTDA), 111 Thailand Science Park, Phahonyothin, Khlong Nueng, Khlong Luang, Pathum Thani 12120, Thailand*

[b] *Department of Materials Science and Engineering, Texas A&M University, College Station, TX 77843-3003, USA*

[c] *Vidyasirimedhi Institute of Science and Technology, Wang Chan, Rayong 21210, Thailand*

[d] *Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand*

1. The metal clusters on pristine and defective graphenes

The optimized configurations and their corresponding E_{ad} of metal tetramers deposited on PG and DG are presented in Figure S1 to S4.

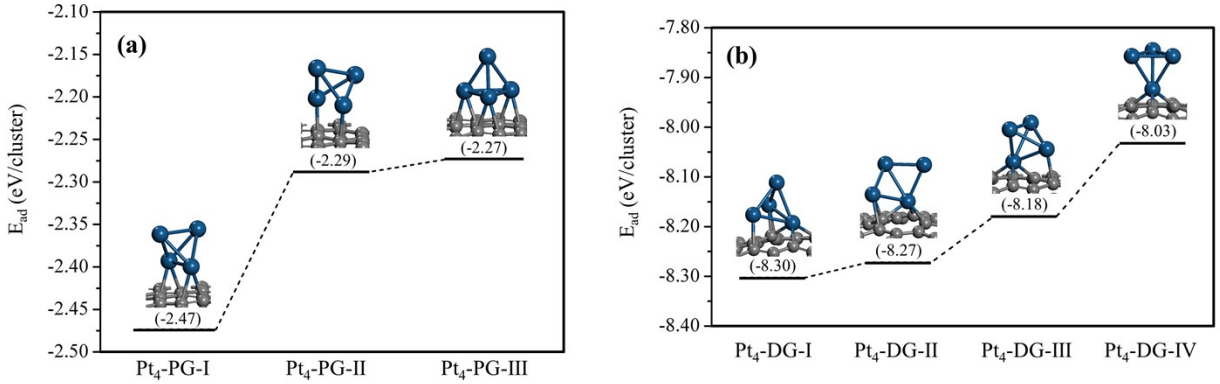

Figure S1. E_{ad} profiles and corresponding structures of (a) Pt_4-PG and (b) Pt_4-DG

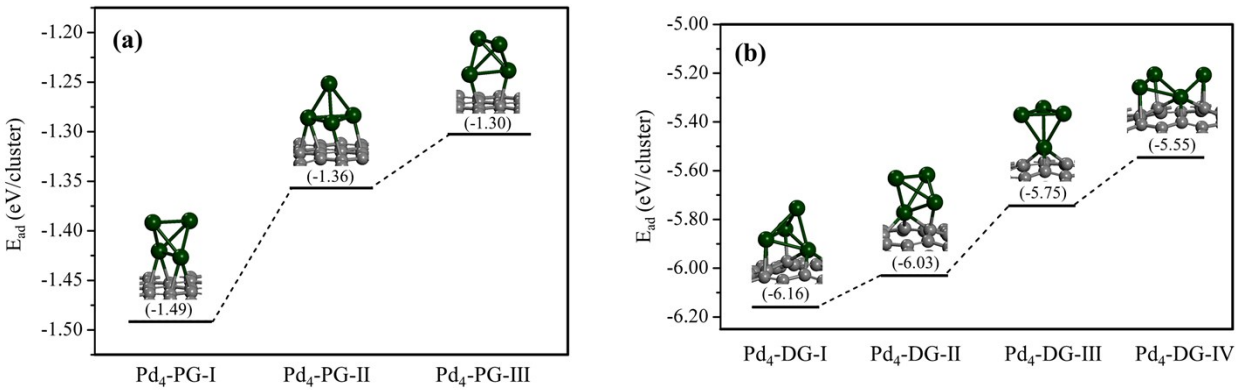

Figure S2. E_{ad} profiles and corresponding structures of (a) Pd_4-PG and (b) Pd_4-DG

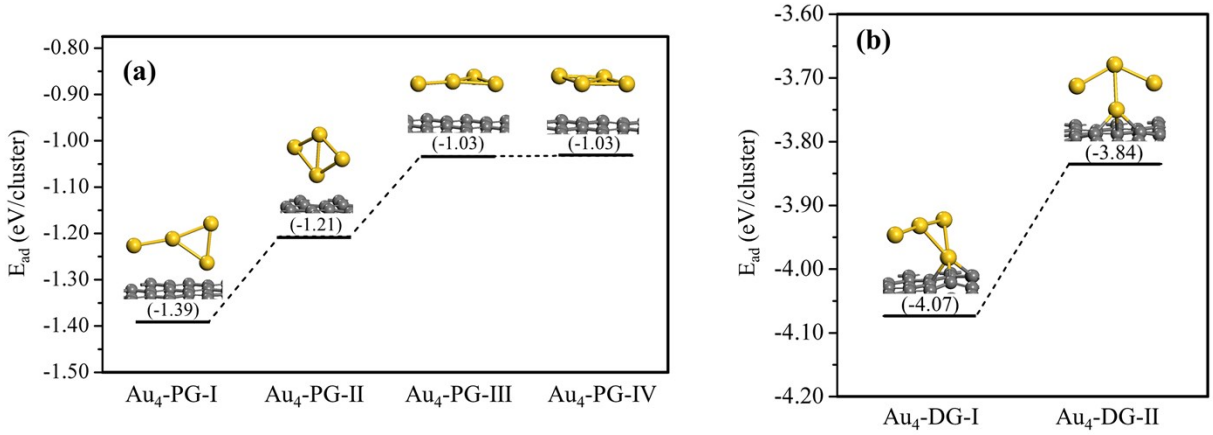

Figure S3. E_{ad} profiles and corresponding structures of (a) Au_4-PG and (b) Au_4-DG

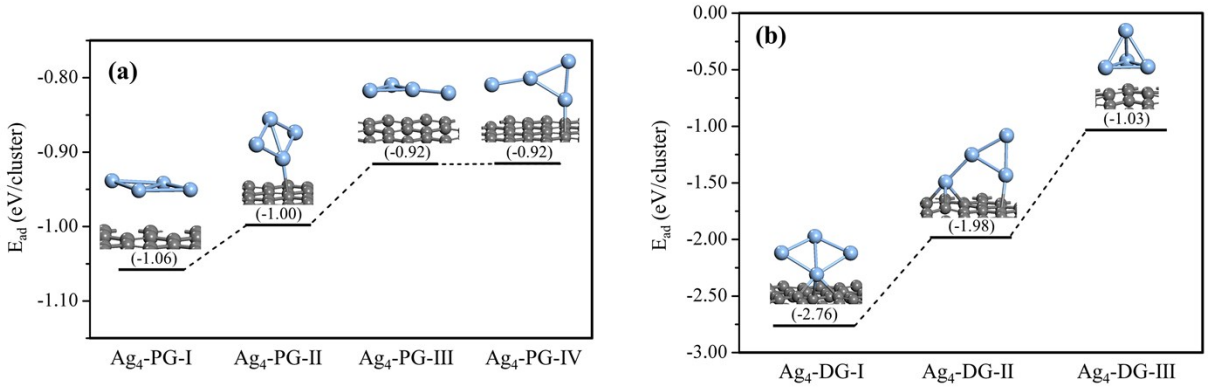

Figure S4. E_{ad} profiles and corresponding structures of (a) Ag_4-PG and (b) Ag_4-DG

2. Electronic charge properties

PDOSs of PG, DG and isolated m-xylene are shown in Figure S5 (a) to (c), respectively. PDOSs of *m*-xylene structures in gas phase and *m*-xylene adsorbed on four substrates are compared in Figure S6.

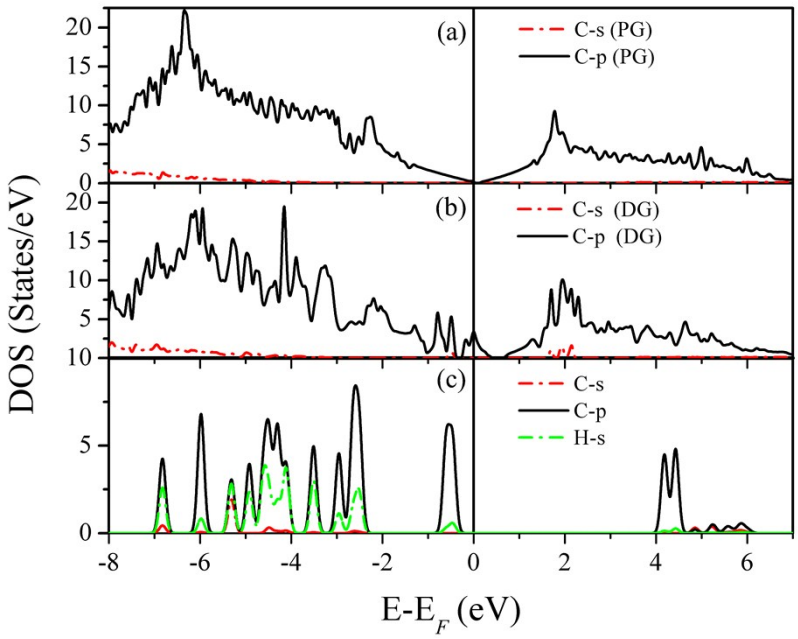

Figure S5. Projected density of states (PDOSs) of (a) PG, (b) DG and (c) isolated *m*-xylene

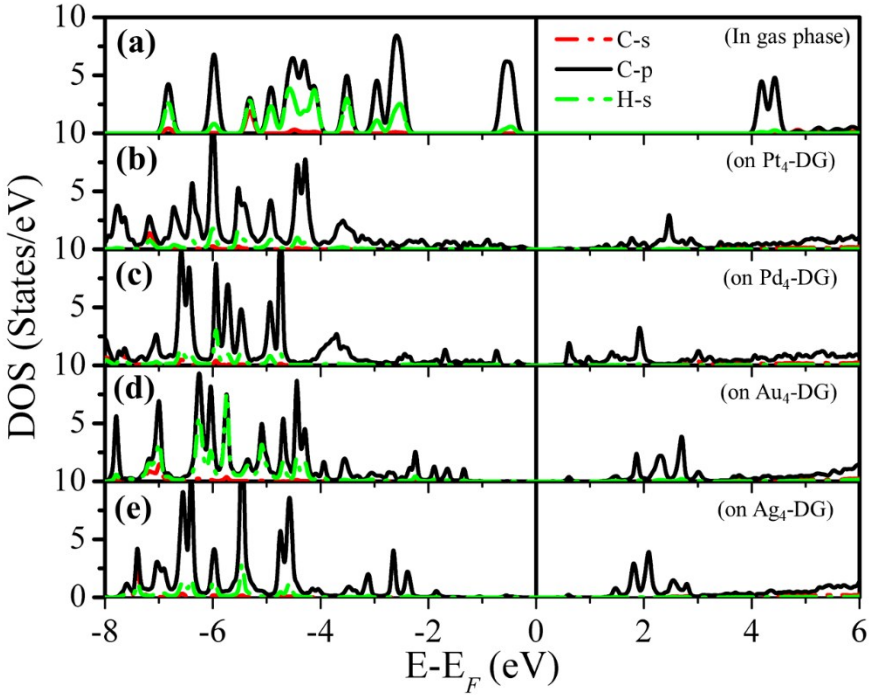

Figure S6. Comparison projected density of states (PDOSs) of *m*-xylene structures in (a) gas phase (b) *m*-xylene/Pt_4-DG, (c) *m*-xylene/Pd_4-DG, (d) *m*-xylene/Au_4-DG and (e) *m*-xylene/Ag_4-DG.