A Light-Driven Modulation of Electric Conductance through Adsorption of Azobenzene onto Silicon-Doped and Pyridine-Like N3-Vacancy Graphene

Jun Zhao[a,b], Chunyan Liu[a], Jing Ma[a,*]

[a]*School of Chemistry and Chemical Engineering, Institute of Theoretical and Computational Chemistry, Key Laboratory of Mesoscopic Chemistry of MOE, Nanjing University, Nanjing 210093, P. R. China;*

[b]*School of Science, Nanjing University of Posts and Telecommunications, Nanjing 210023, P. R. China*

The optical absorbance computational details:

The imaginary part $\varepsilon_2(\omega)$ of the dielectric function is calculated by:

$$\varepsilon_2(\omega) = \frac{4\pi^2 e^2}{\Omega} \lim_{q\to 0} \frac{1}{q^2} \sum_{c,v,k} 2\omega_k \delta^*(\varepsilon_{ck} - \varepsilon_{vk} - \omega) \times \left\langle \mu_{ck+e_{\alpha q}} \middle| \mu_{vk} \right\rangle \left\langle \mu_{ck+e_{\beta q}} \middle| \mu_{vk} \right\rangle \quad (1)$$

where the indices *c* and *v* refer to conduction and valence band states, respectively.

The real part $\varepsilon_1(\omega)$ then can be obtained from the Kramer-Kroning transformation. Moreover, the frequency-dependent optical absorbance $\alpha(\omega)$ is estimated by:

$$\alpha(\omega) = \sqrt{2}\omega[\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} - \varepsilon_1(\omega)]^{\frac{1}{2}} \quad (2)$$

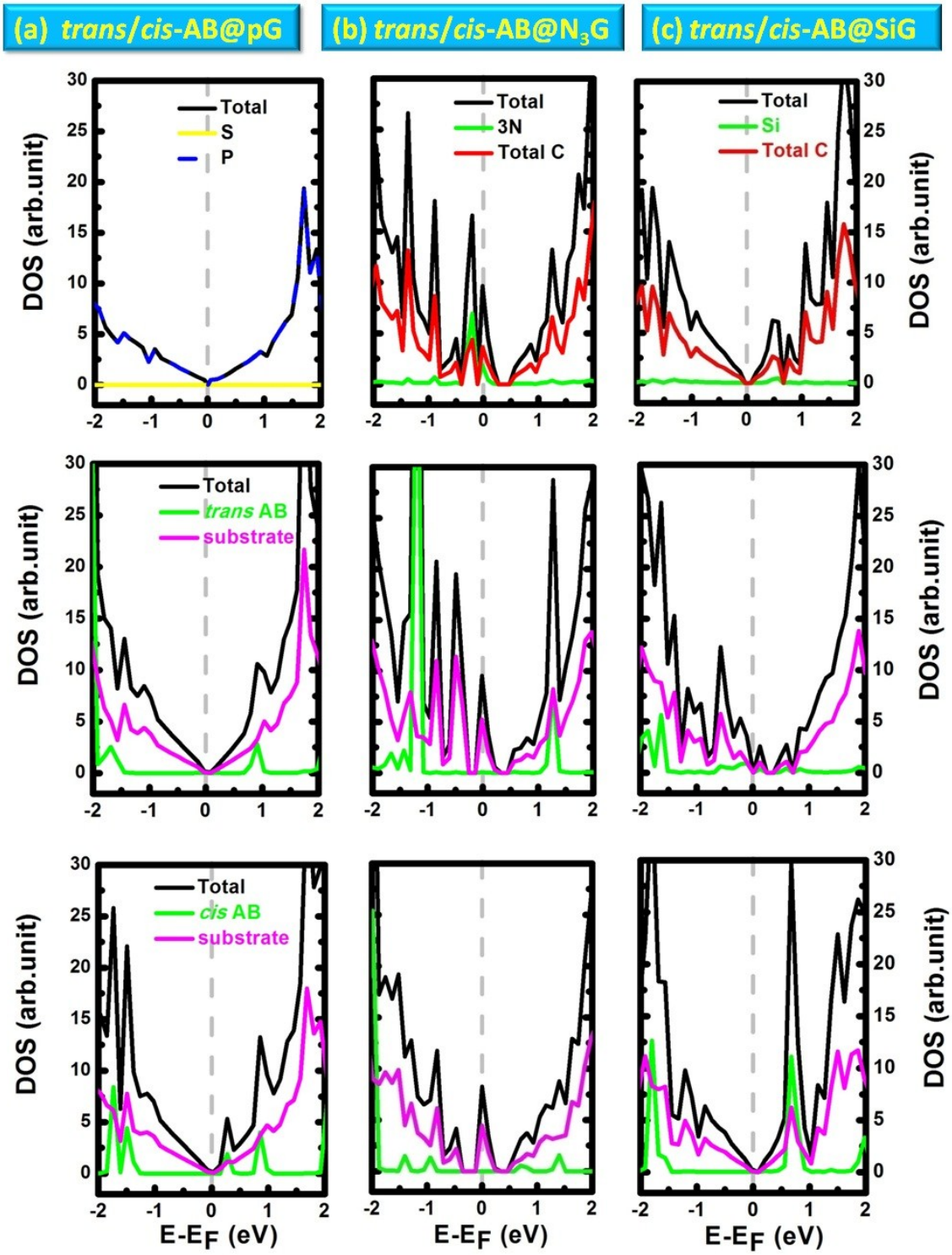

Figure S1. Density of states (DOS) for *trans*/*cis*-AB adsorbed onto (a) pG, (b) N_3G and (c) SiG. The Fermi level is set to zero and indicated by the dashed line.

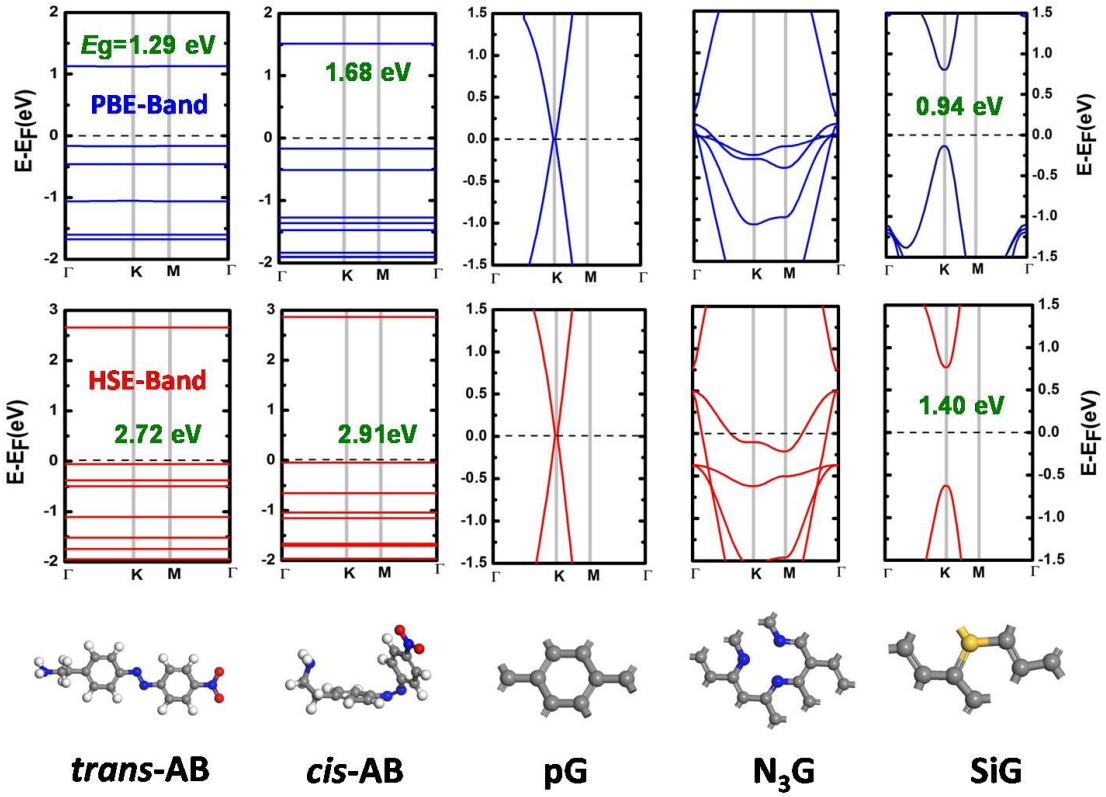

Figure S2. The comparison of the band structures calculated by PBE and HSE06 functionals for isolated *trans*/*cis* AB isomer, pG, N_3G and SiG with smaller unit cell, respectively.

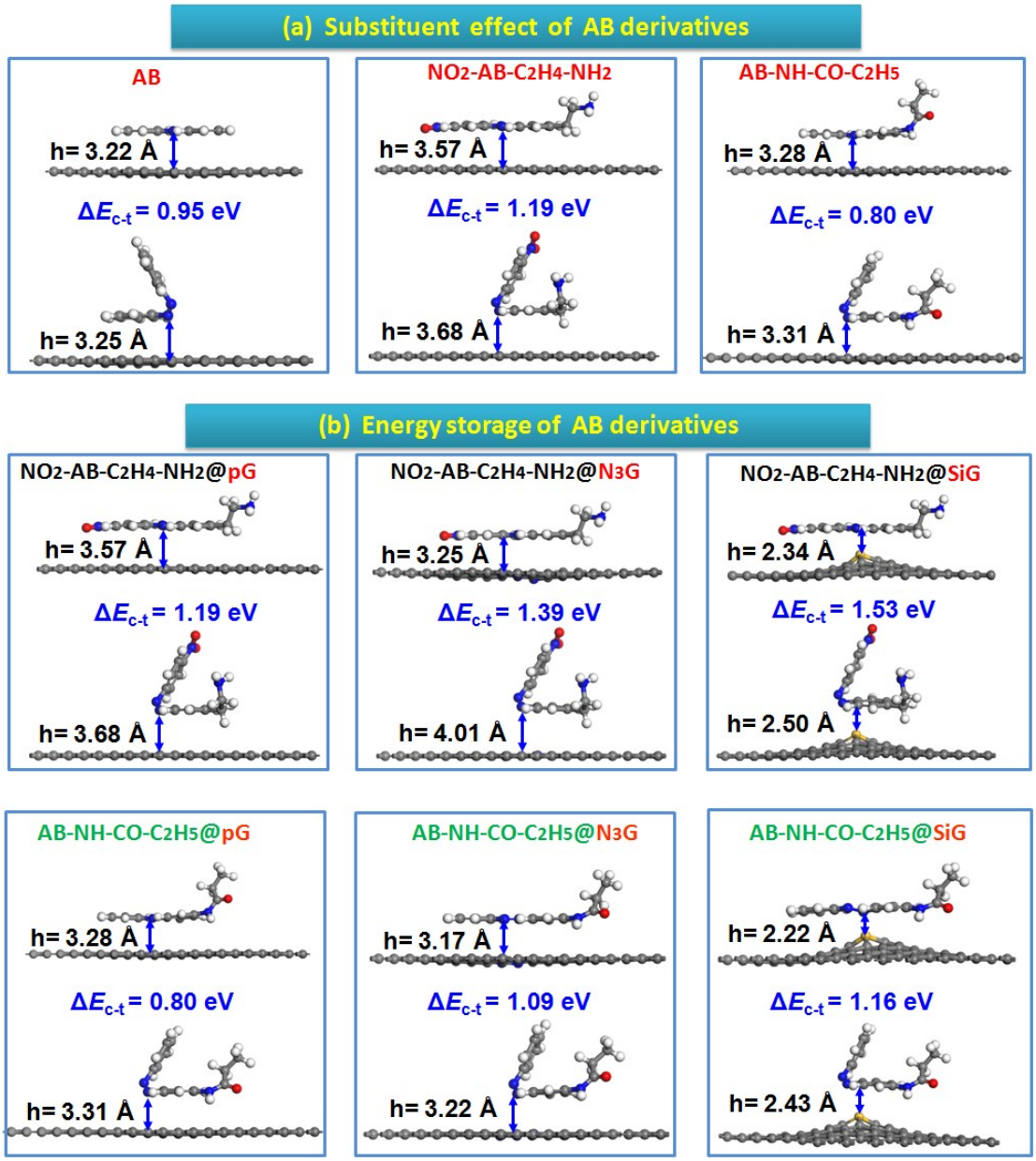

Figure S3. (a) The optimized structures of unsubstituted azobenzene (AB), NO_2-AB-C_2H_4-NH_2 and AB-NH-CO-C_2H_5 adsorbed onto pG substrate. (b) The optimized structures of NO_2-AB-C_2H_4-NH_2 and AB-NH-CO-C_2H_5 adsorbed onto pG, N_3G and SiG substrates, respectively. The adsorption distance (h) and storing energy of each system (ΔEc-t) are also given.