Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2022

Supplementary Information

Effect of co-adsorption of small molecules in air on property of penta-graphene and their proton transfer

Kaixuan Jin[a,b], *Kun Lu*[a,b] *and Xiaojie Liu*[a,b,*]

[a]Center for Quantum Sciences and School of Physics, Northeast Normal University, Changchun, 130117, China.

[b]Center for Advanced Optoelectronic Functional Materials Research, and Key Laboratory of UV Light-Emitting Materials and Technology of Ministry of Educations, Northeast Normal University, Changchun, 130024, China.

Email: liuxj100@nenu.edu.cn

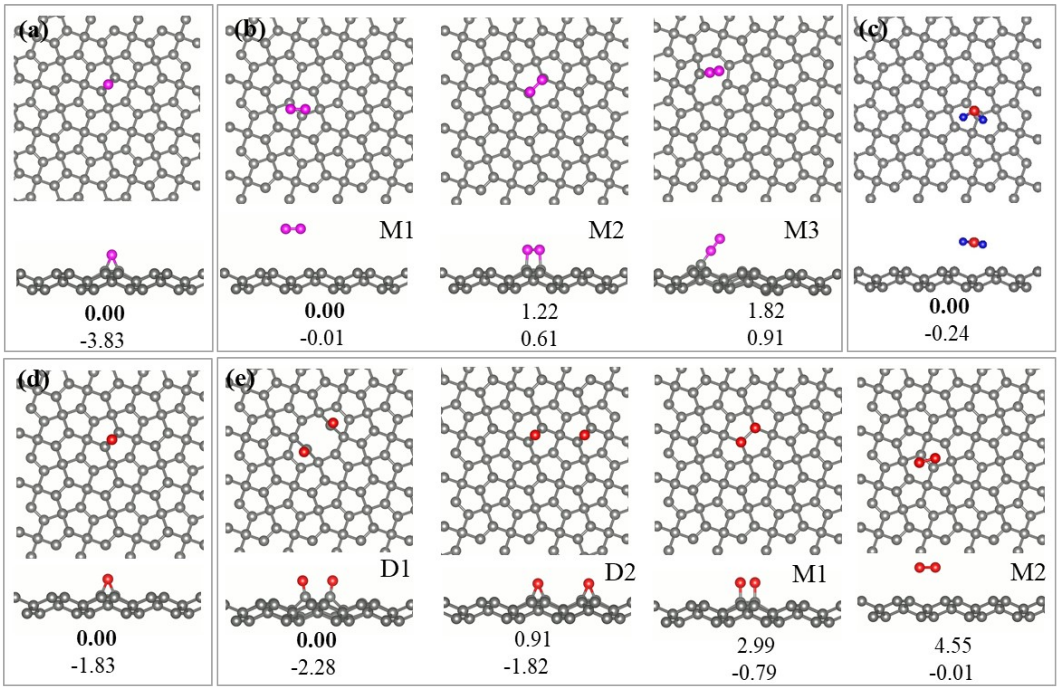

Figure S1. (a) Geometries of atomic N on penta-graphene. (b) Isomers of N_2 molecule on penta-graphene. (c) Geometries of water molecule on penta-graphene. (d) Geometries of atomic O on penta-graphene. (e) Isomers of O_2 molecule on penta-graphene. The relatively energies with the lowest energy isomers as well as adsorption energies are also listed in each structure. The gray, pink, blue and red balls represent the carbon, nitrogen, hydrogen and oxygen atoms, respectively.

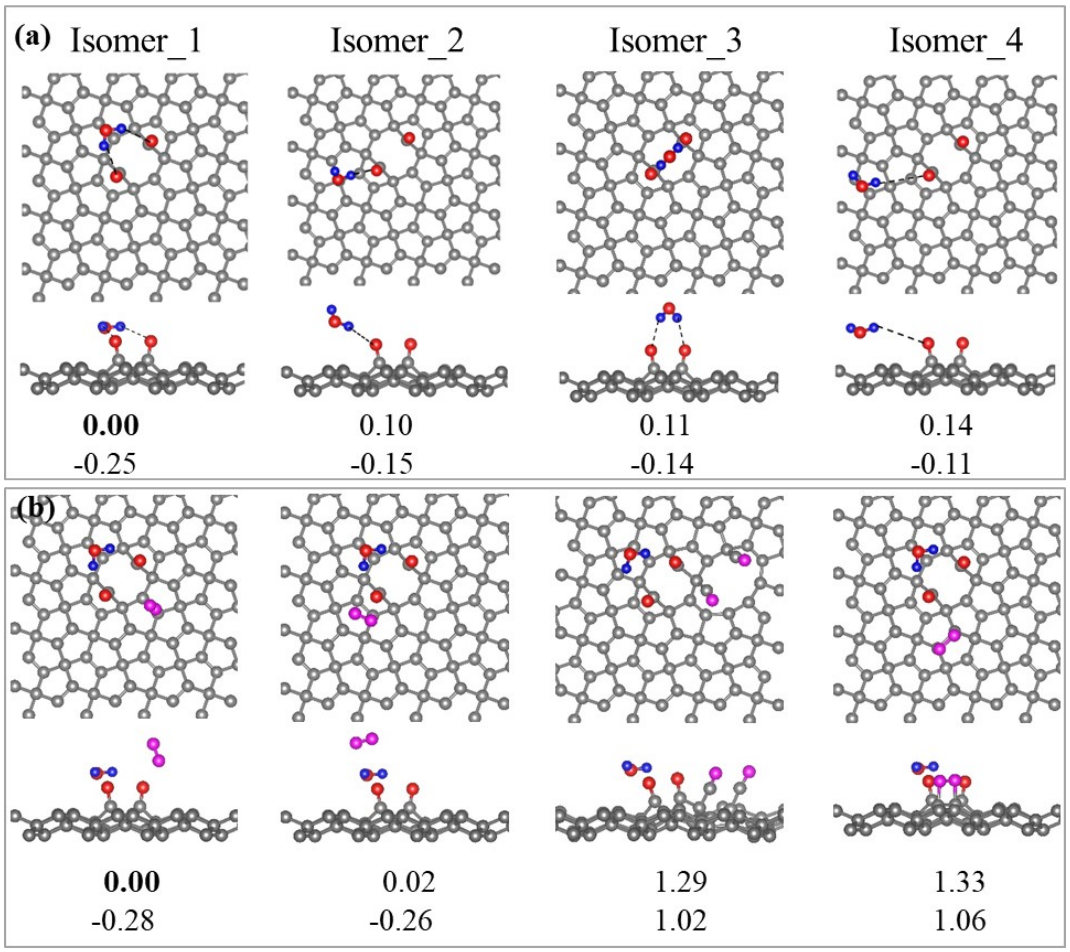

Figure S2. (a) Geometries of H_2O molecule on oxidized penta-graphene (O/p-Gra). (b) Geometries of N_2 and H_2O molecules co-adsorption on oxidized penta-graphene (O/p-Gra). The relatively energies with the lowest energy isomers as well as adsorption energies are also listed in each structure. The adsorption energy is defined as $E_{ads} = E_{total} - E_{O/p\text{-}Gra} - E_{gas}$.