Supplementary Material

Molecular Interactions of MeOH and EtOH with Black Phosphorus Monolayer: A Periodic Density Functional Study

Mehdi Ghambarian¹, Mohammad Ghashghaee²*, Zahra Azizi³, Mahboobeh Balar²,⁴

¹ Gas Conversion Department, Faculty of Petrochemicals, Iran Polymer and Petrochemical Institute, P.O. Box 14975-112, Tehran, Iran
² Faculty of Petrochemicals, Iran Polymer and Petrochemical Institute, P.O. Box 14975-112, Tehran, Iran
³ Department of Chemistry, Karaj Branch, Islamic Azad University, P.O. Box 31485-313, Karaj, Iran
⁴ Young Researchers and Elite Club, Karaj Branch, Islamic Azad University, Karaj, Iran

* Corresponding author. Tel.: +98 21 48662481; fax: +98 21 44787032. E-mail address: m.ghashghaee@ippi.ac.ir
Figure S1. Optimized geometries of the adsorption complexes at the PBEPBE/6-31G* level of theory. The orange balls represent phosphorus, the grey balls represent carbon, the red balls show oxygen, and the smaller white atoms are hydrogen.
Figure S1 (Contd.)
Figure S2. Calculated band structure for the parent bulk black phosphorus model.