Supplementary Material

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

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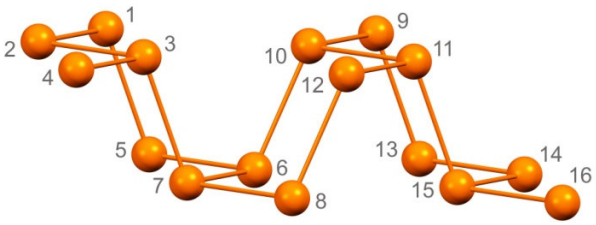
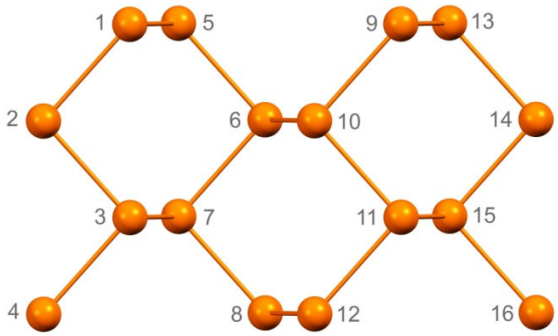
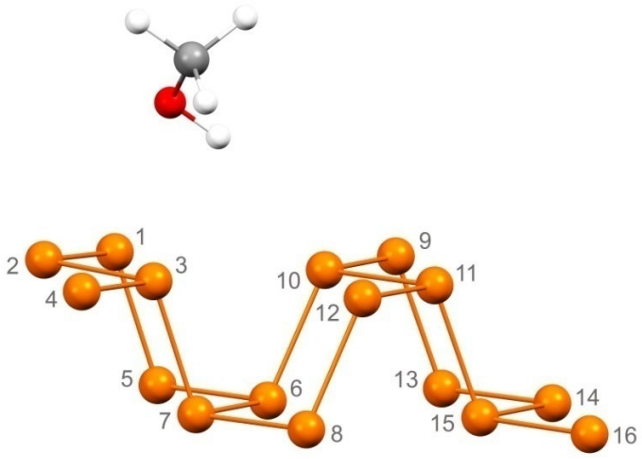


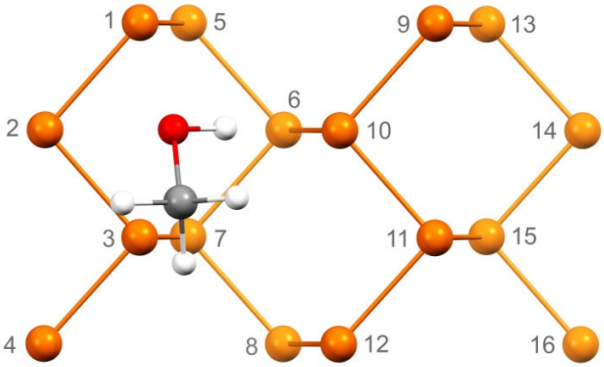
BPML (Side view)



BPML (Top view)

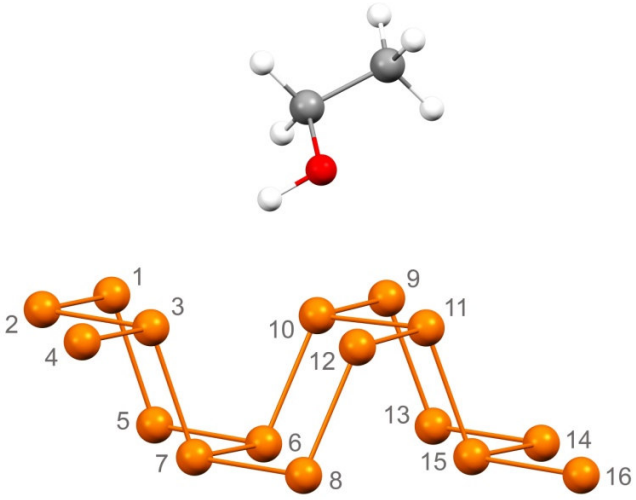


BP-MeOH (Side view)

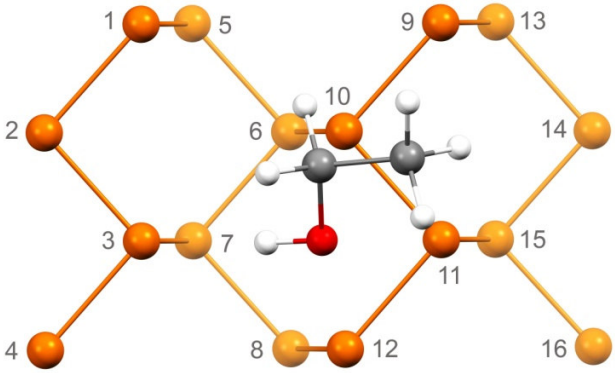


BP-MeOH (Top view)

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.



BP-EtOH (Side view)



BP-EtOH (Top view)

Figure S1 (Contd.)

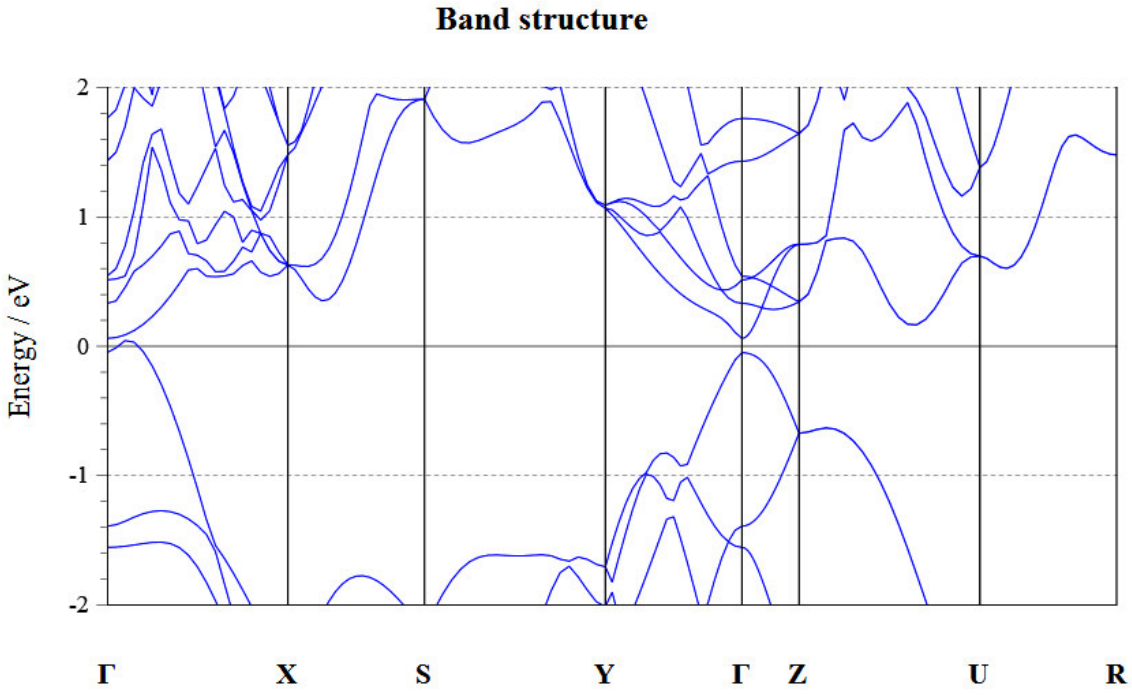


Figure S2. Calculated band structure for the parent bulk black phosphorus model.