

Electronic supplementary information

Density Functional Theory Study on the Underwater Adhesion of Catechol onto a Graphite

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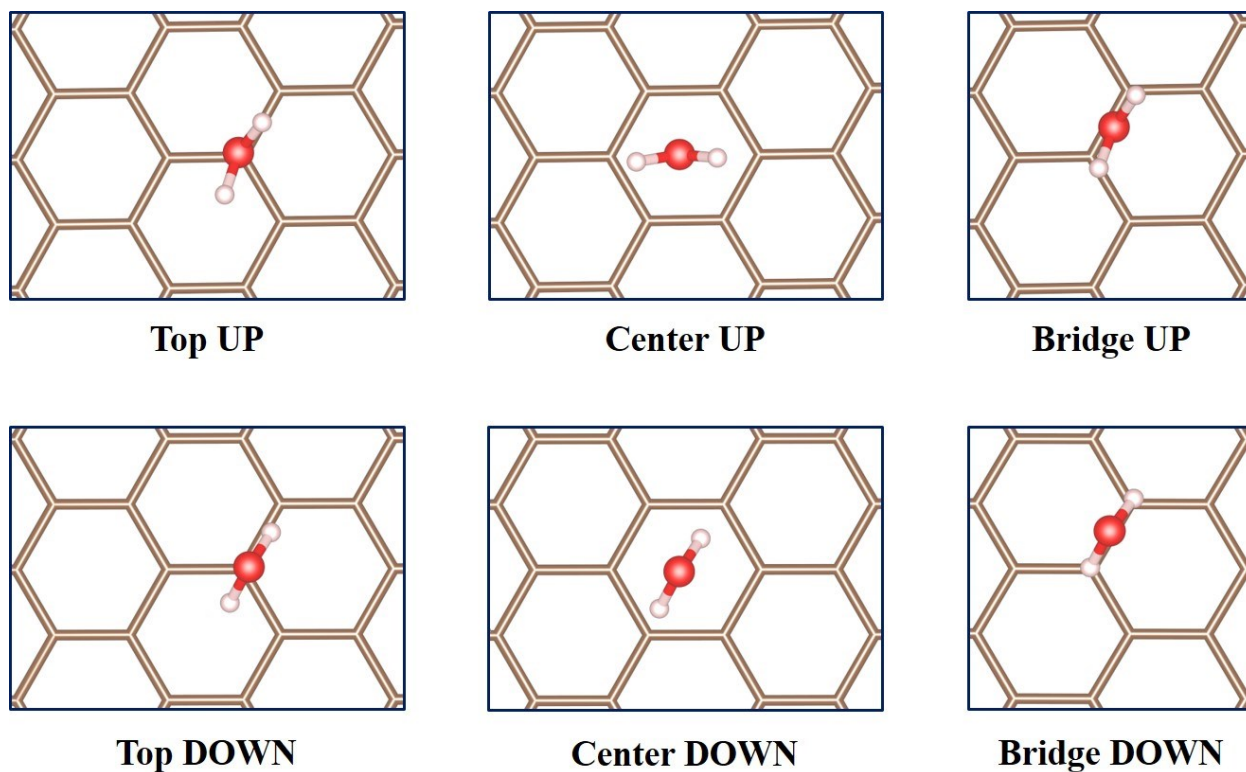


Figure S1. Optimized geometries of water molecules adhered on three different locations of a dry graphite surface: on top of a C atom (top), on top of the center of a hexagonal ring of C (center), and on top of a bridge site of C-C bond (bridge). For three locations, we consider two orientations where the hydroxyl groups of water point up from and down toward the graphite surface. Only the top layer of the graphite is shown. The red and white balls represent the O and H atoms of the water molecule.

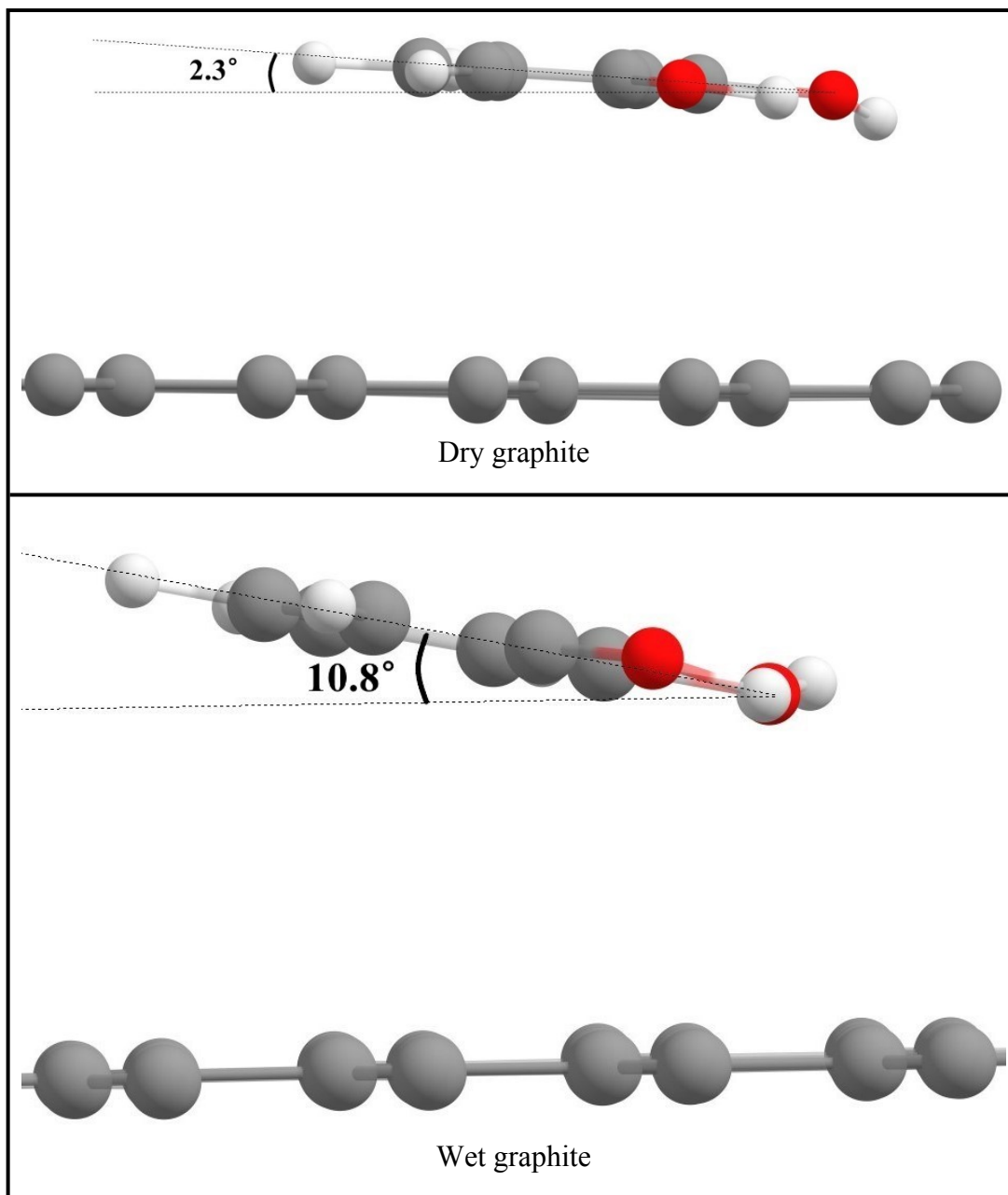


Figure S2. Tilt angles of catechols adhered to the dry (top) and wet graphite (bottom) surfaces.

For the wet graphite, water molecules are not shown for visual clarity.