Supporting information for

"A dispersion-corrected DFT study on adsorption of battery active materials anthraquinone and its derivatives on monolayer graphene and *h*-BN"

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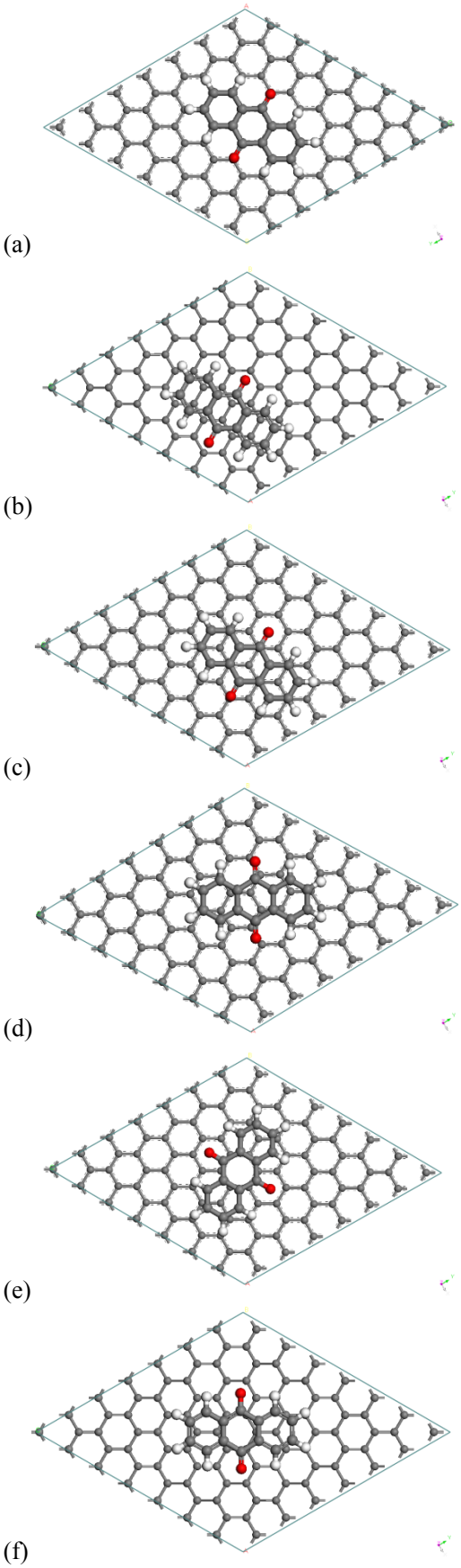

Figure S1. Equilibrium geometries of an AQ molecule on different adsorption sites of a graphene nanosheet: (a) AA, (b) BP, (c) AB, (d) BS, (e) Cross and (f) SC.

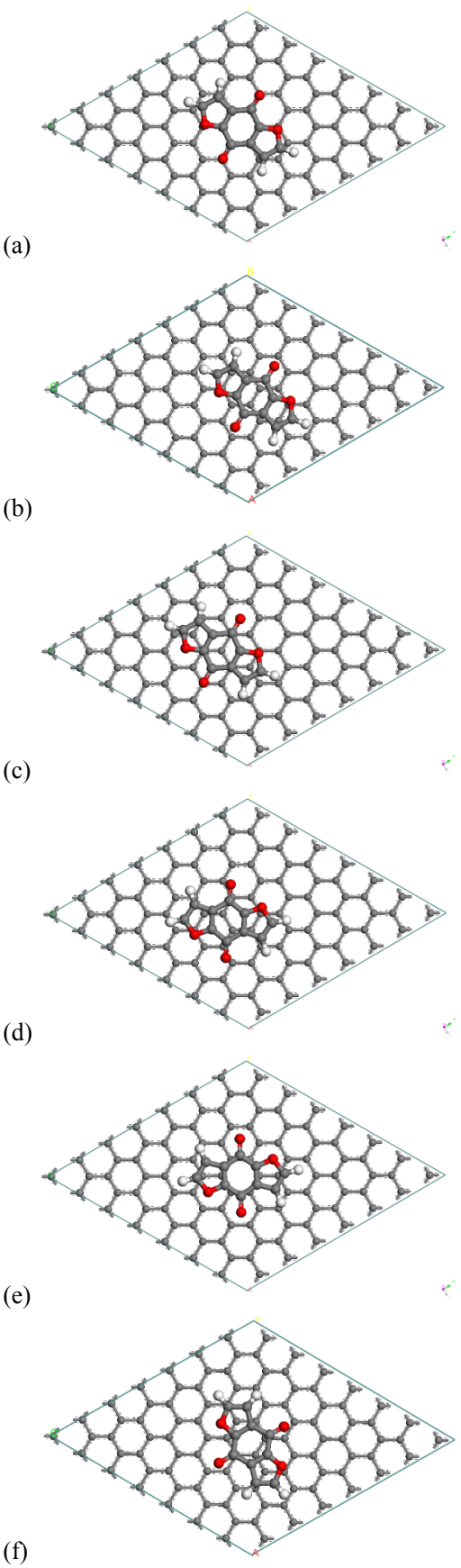

Figure S2. Equilibrium geometries of a BFFD molecule adsorbed on different adsorption sites of a graphene nanosheet: (a) AA, (b) BP, (c) AB, (d) BS, (e) Cross and (f) SC.

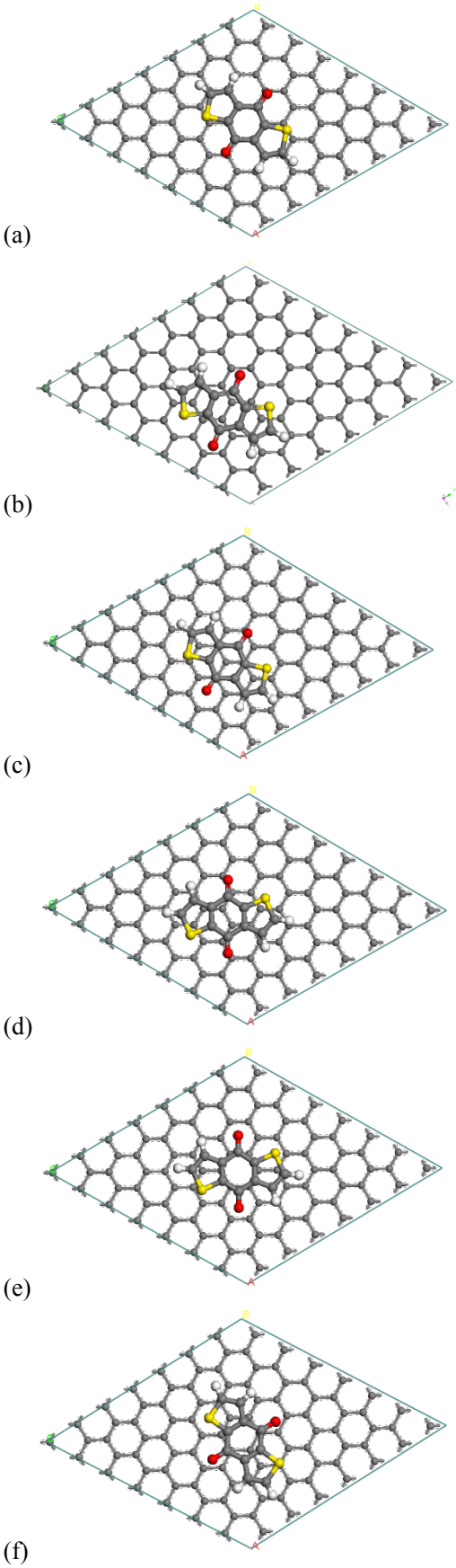

Figure S3. Equilibrium geometries of a BDTD molecule adsorbed on different sites of a graphene nanosheet: (a) AA, (b) BP, (c) AB, (d) BS, (e) Cross and (f) SC.

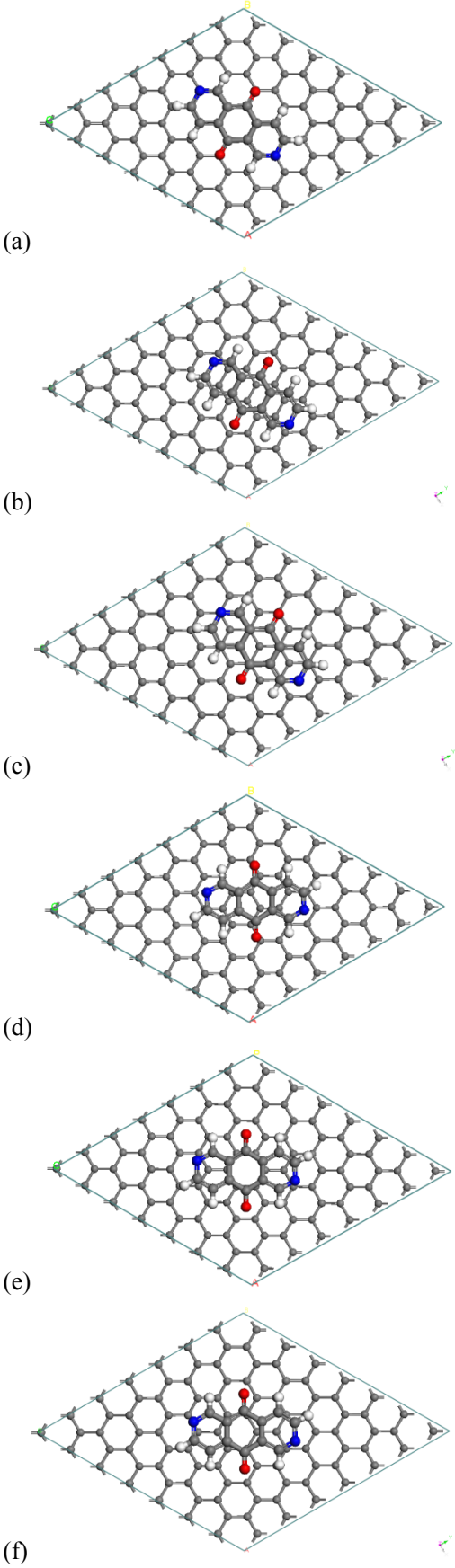

Figure S4. Equilibrium geometries of a PID molecule adsorbed on different adsorption sites of a graphene nanosheet: (a) AA, (b) BP, (c) AB, (d) BS, (e) Cross and (f) SC.

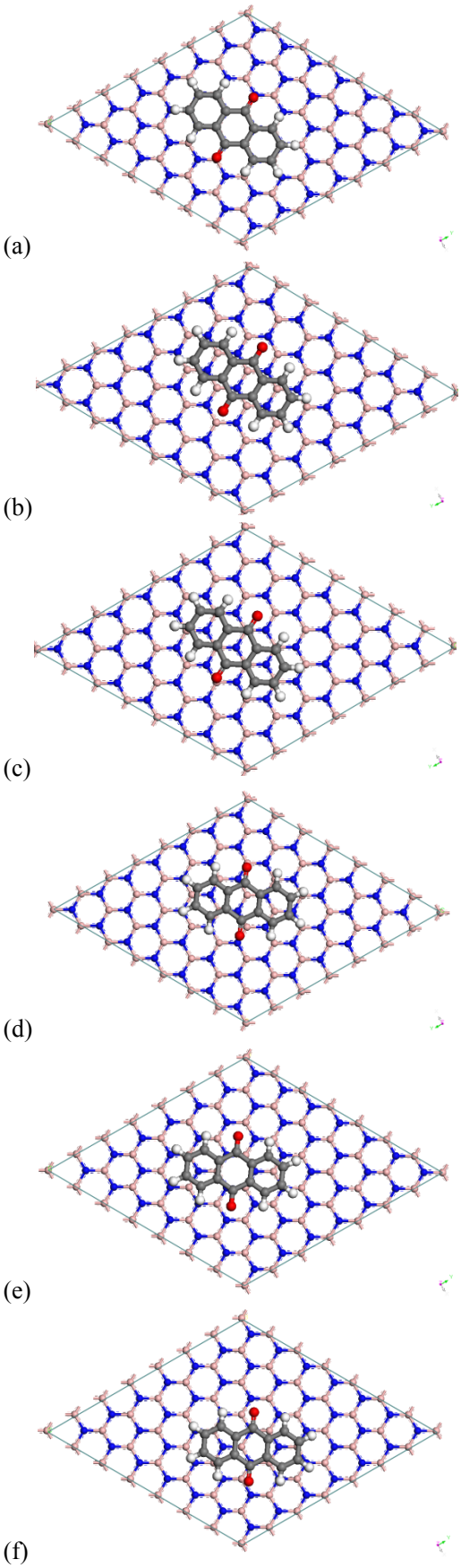

Figure S5. Equilibrium geometries of an AQ molecule adsorbed on different adsorption sites of a BN nanosheet: (a) AA, (b) BP, (c) AB, (d) BS, (e) Cross and (f) SC.

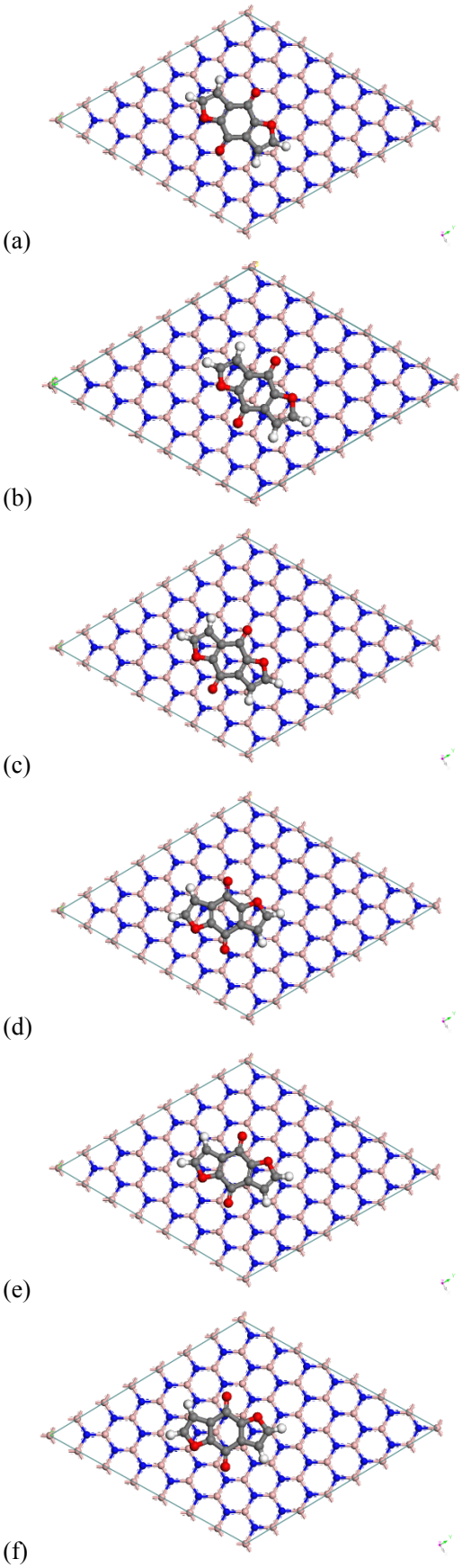

Figure S6. Equilibrium geometries of a BFFD molecule adsorbed on different adsorption sites of a BN nanosheet: (a) AA, (b) BP, (c) AB, (d) BS, (e) Cross and (f) SC.

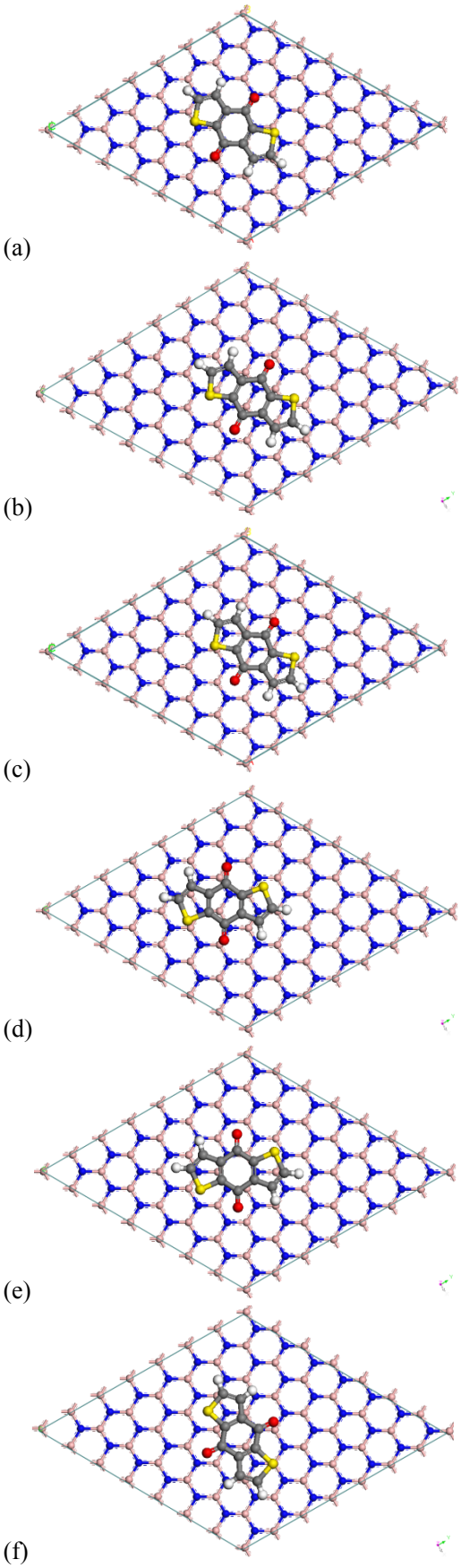

Figure S7. Equilibrium geometries of a BDTD molecule adsorbed on different adsorption sites of a BN nanosheet: (a) AA, (b) BP, (c) AB, (d) BS, (e) Cross and (f) SC.

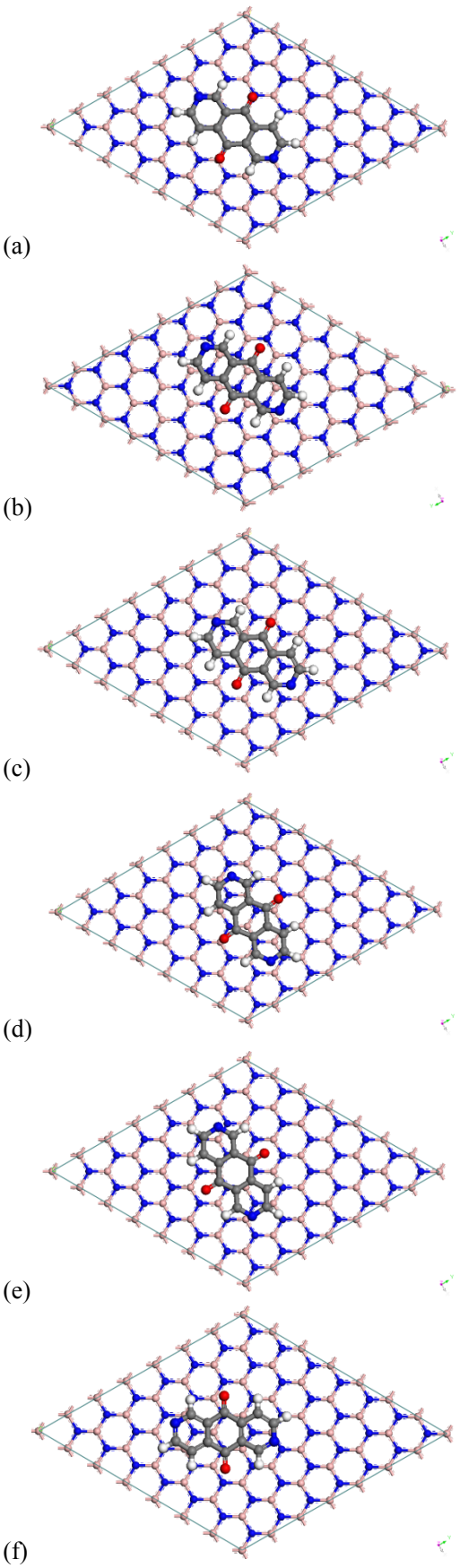

Figure S8. Equilibrium geometries of a PID molecule adsorbed on different adsorption sites of a BN nanosheet: (a) AA, (b) BP, (c) AB, (d) BS, (e) Cross and (f) SC.