

Supporting Information

for

DFT and TD-DFT Studies on the Electronic and Optical Properties of Explosive Molecules Adsorbed on Boron Nitride and Graphene Nano Flakes

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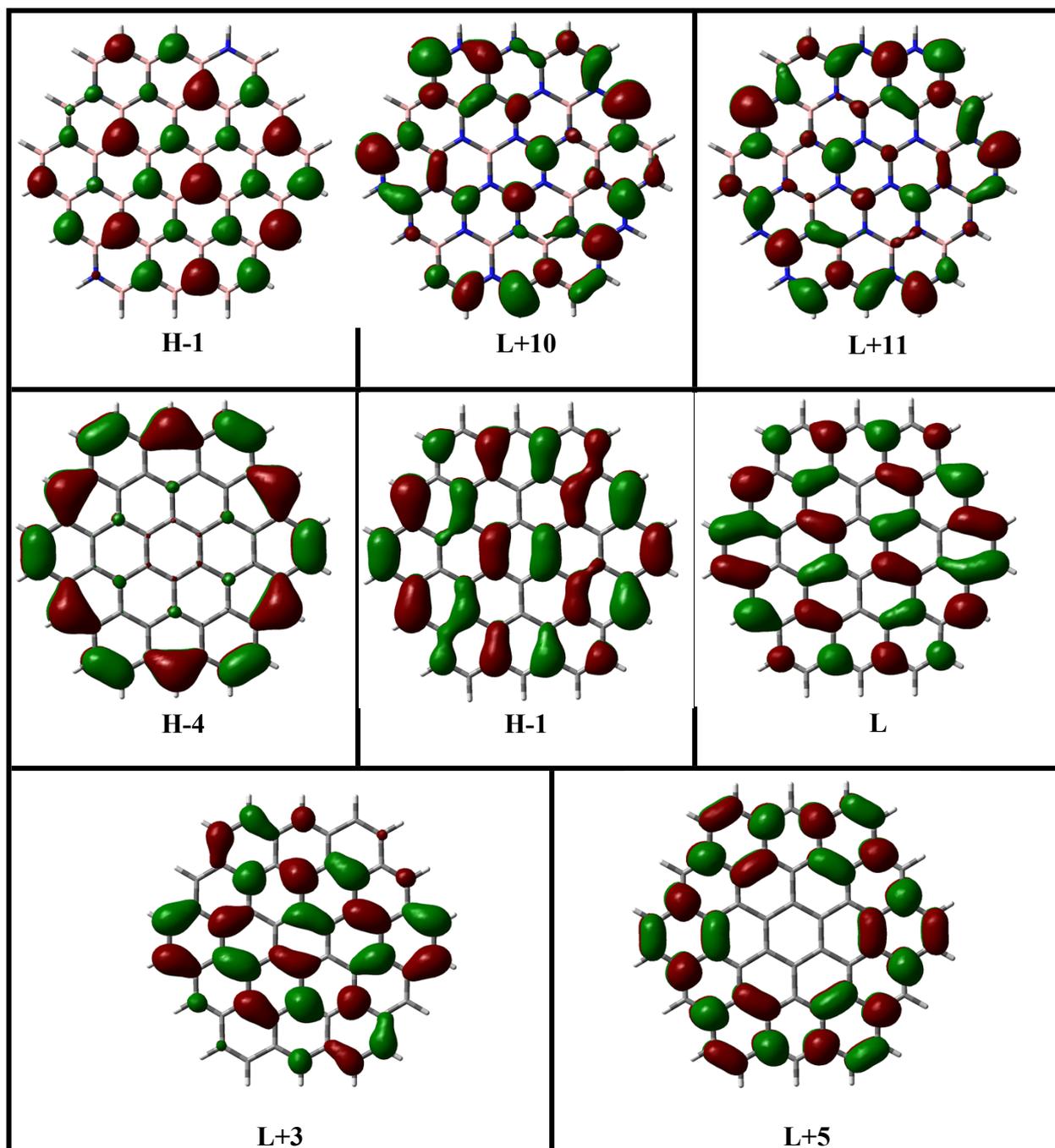


Figure S1. Frontier molecular orbitals involved in the vertical excitation of BN and G flake.

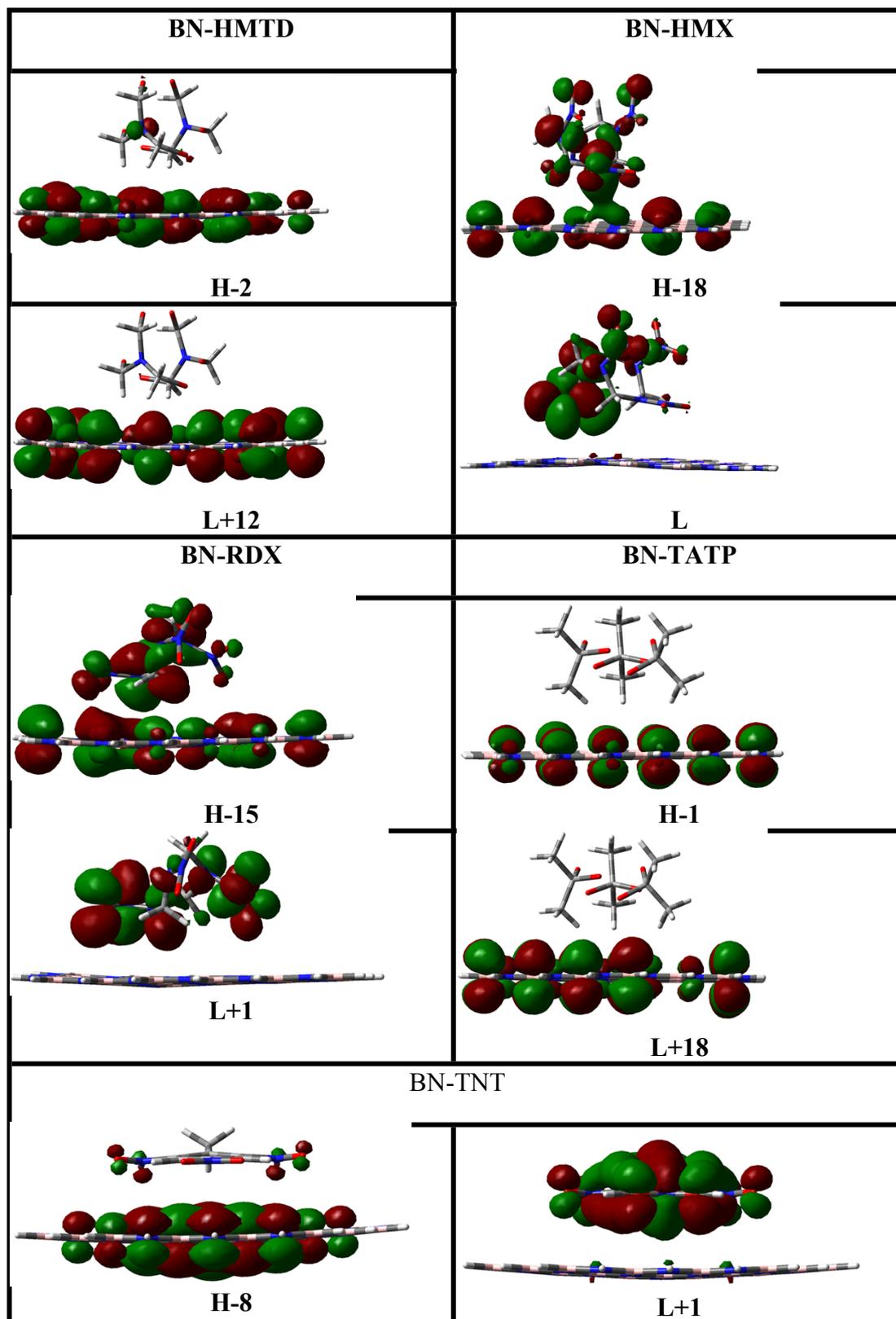


Figure S2. Frontier molecular orbitals involved in the vertical excitation of BN-explosive complexes.

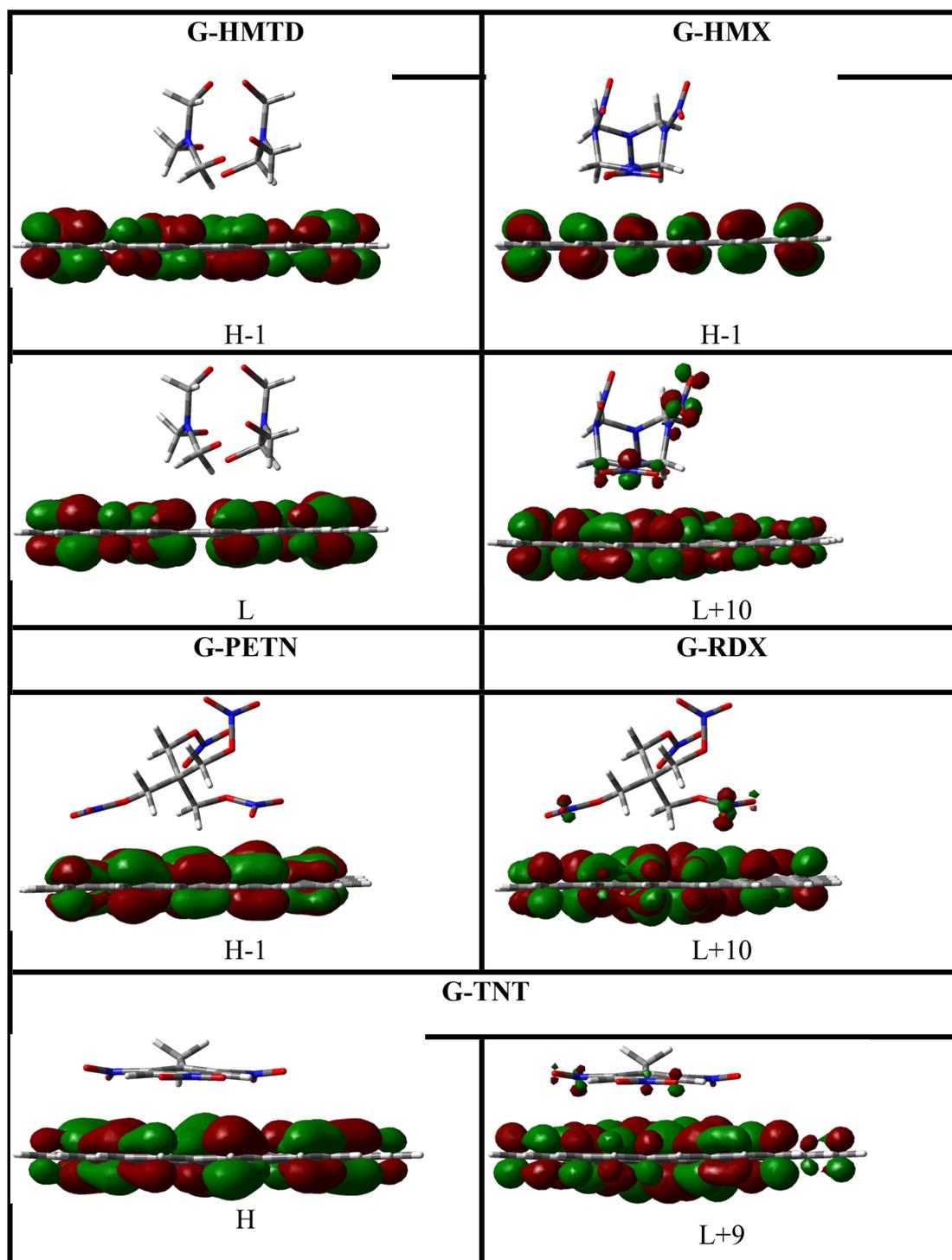


Figure S3. Frontier molecular orbitals involved in the vertical excitation of G-explosive complexes.

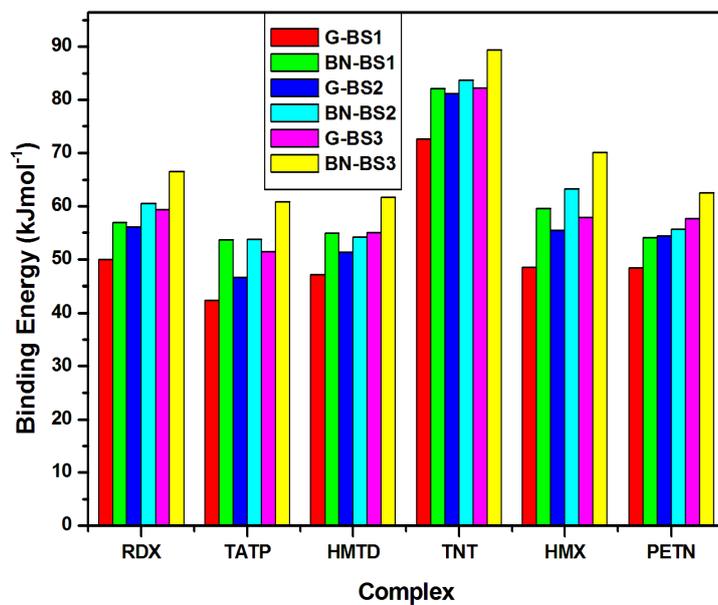


Figure S4. Comparison BE of BN and G-explosive complexes with different basis sets using B3LYP-D/BS1 or BS2 or BS3 (BS1:6-311++G(2d,2p), BS2: 6-311G(2df,2pd) and BS3: cc-pVTZ).

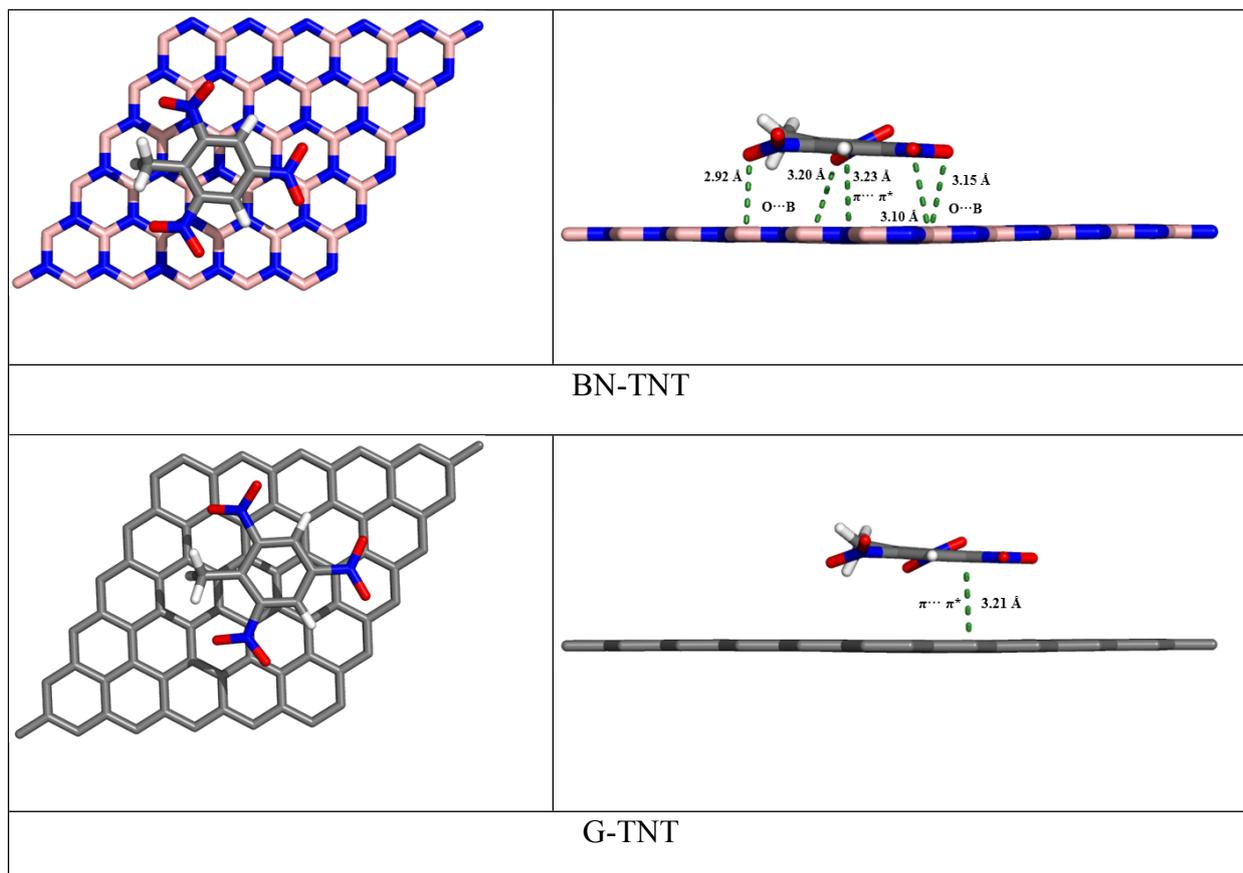


Figure S5. Energy minimized structures of complexes of TNT with 2D periodic BN and G sheets.

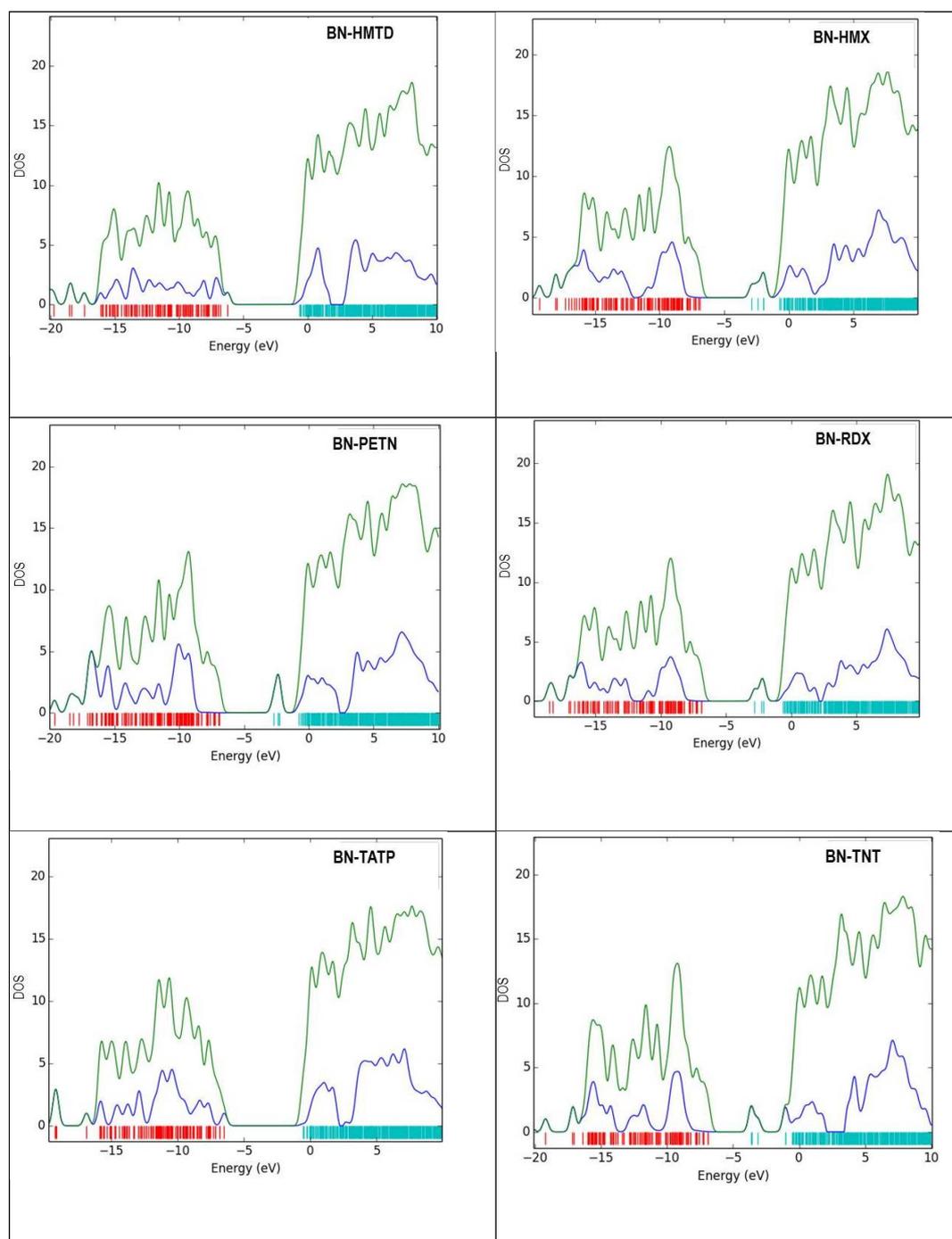


Figure S6. Calculated partial density of states (PDOS) of BN-explosive complexes with B3LYP-D/6-31+G(d,p) level of theory. (Green: BN, Blue: explosive molecule, Red: Occupied MO's, Cyan: Unoccupied MO's).

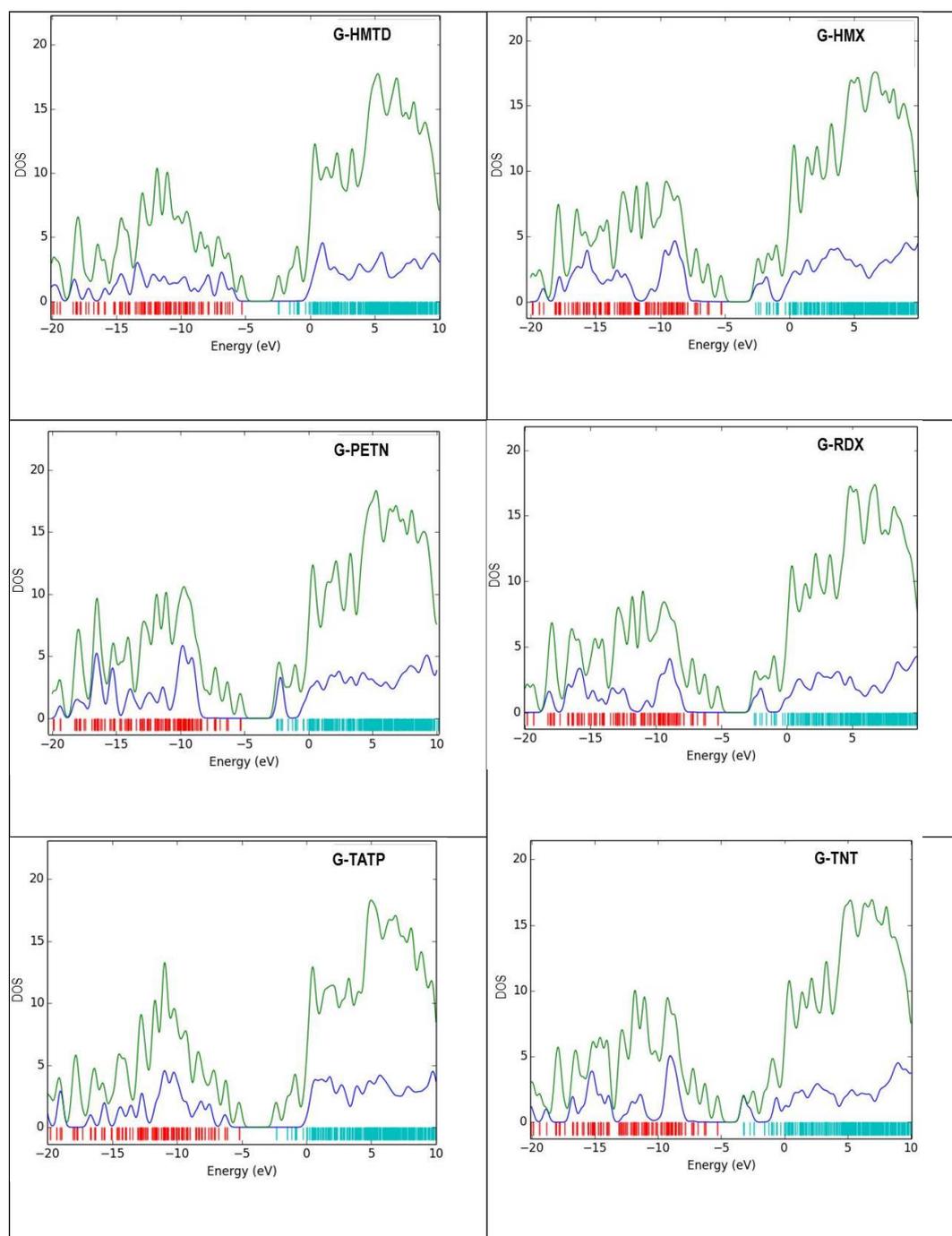


Figure S7. Calculated partial density of states (PDOS) of BN-explosive complexes with B3LYP-D/6-31+G(d,p) level of theory (Green: BN, Blue: explosive molecule, Red: Occupied MO's, Cyan: Unoccupied MO's).

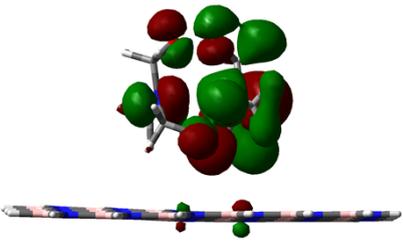
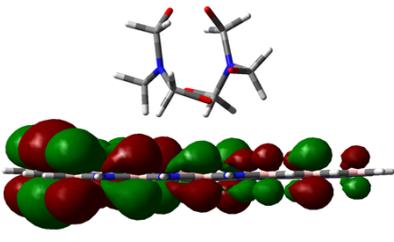
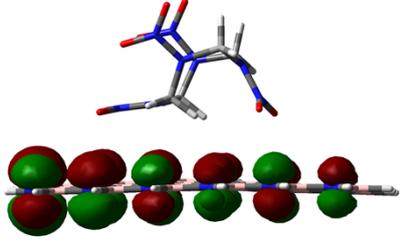
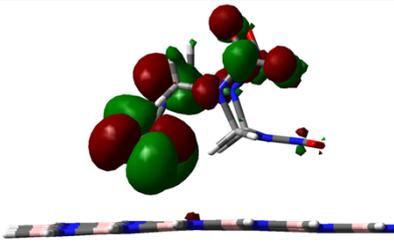
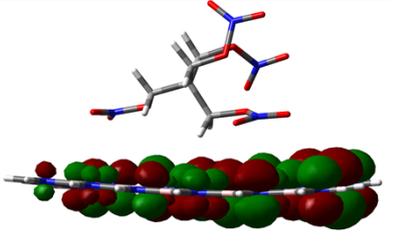
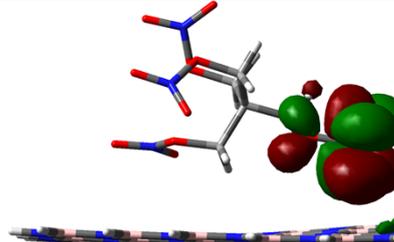
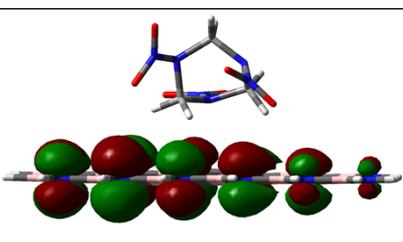
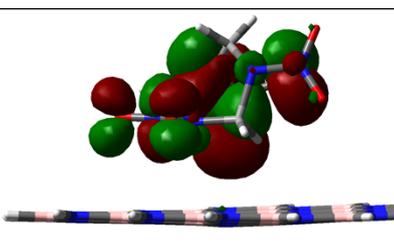
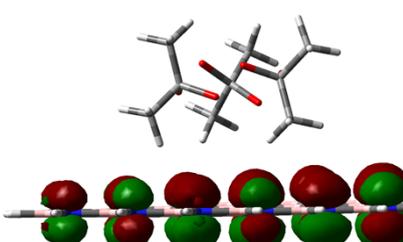
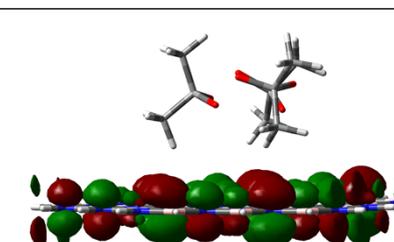
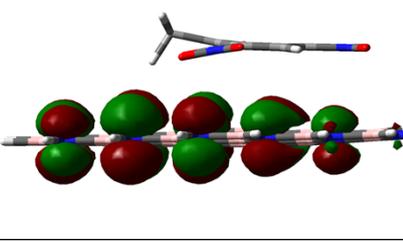
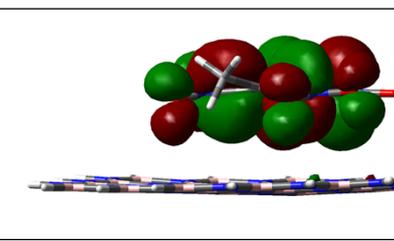
System	HOMO	LUMO
BN-HMTD		
BN-HMX		
BN-PETN		
BN-RDX		
BN-TATP		
BN-TNT		

Figure S8. HOMO and LUMO isosurfaces of BN-explosive complexes at B3LYP-D/6-31+G(d,p) level of theory.

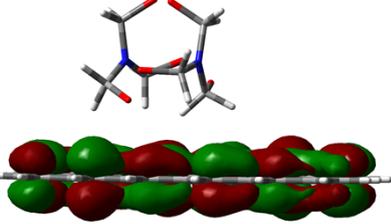
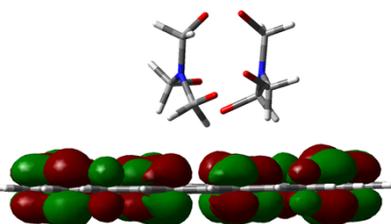
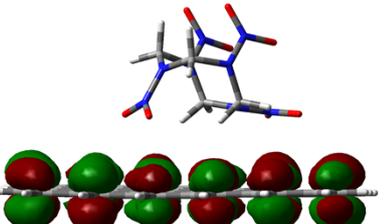
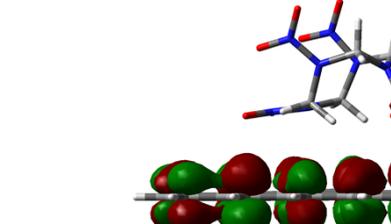
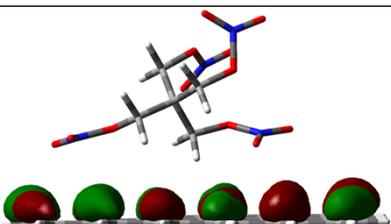
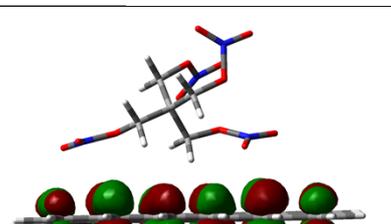
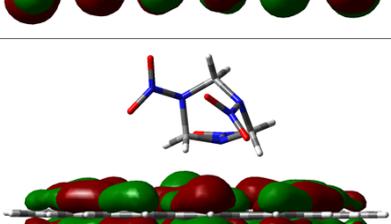
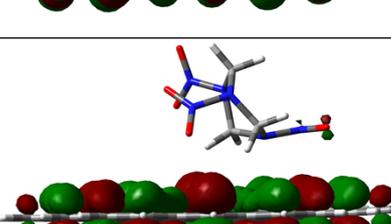
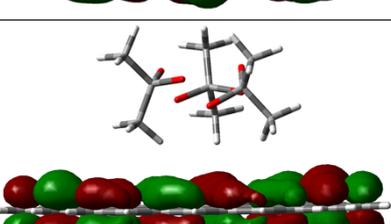
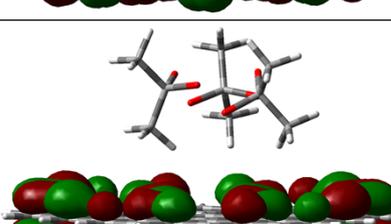
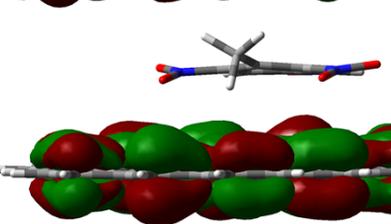
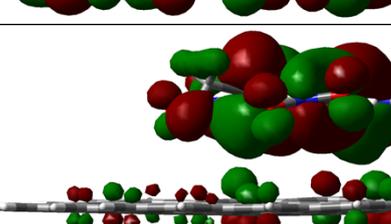
System	HOMO	LUMO
G-HMTD		
G-HMX		
G-PETN		
G-RDX		
G-TATP		
G-TNT		

Figure S9. HOMO and LUMO isosurfaces of G-explosive complexes at B3LYP-D/6-31+G(d,p) level of theory.