Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Supporting Information

Theoretical Insights into the Structural, Electronic, Photocatalytic and Supercapacitor Application of Pentahexoctite

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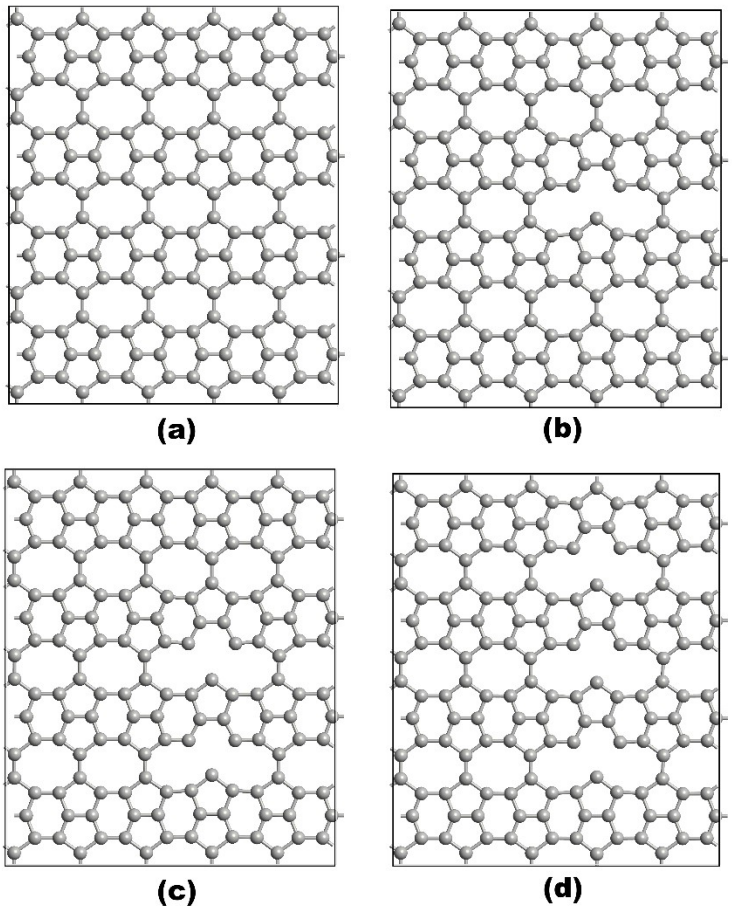

Figure S1: Optimized structure of (a) $4 \times 5 \times 1$ supercells of pristine pentahexoctite, (b) single vacancy, (c) double vacancy and (d) triple vacancy of $4 \times 5 \times 1$ supercells of pristine pentahexoctite.

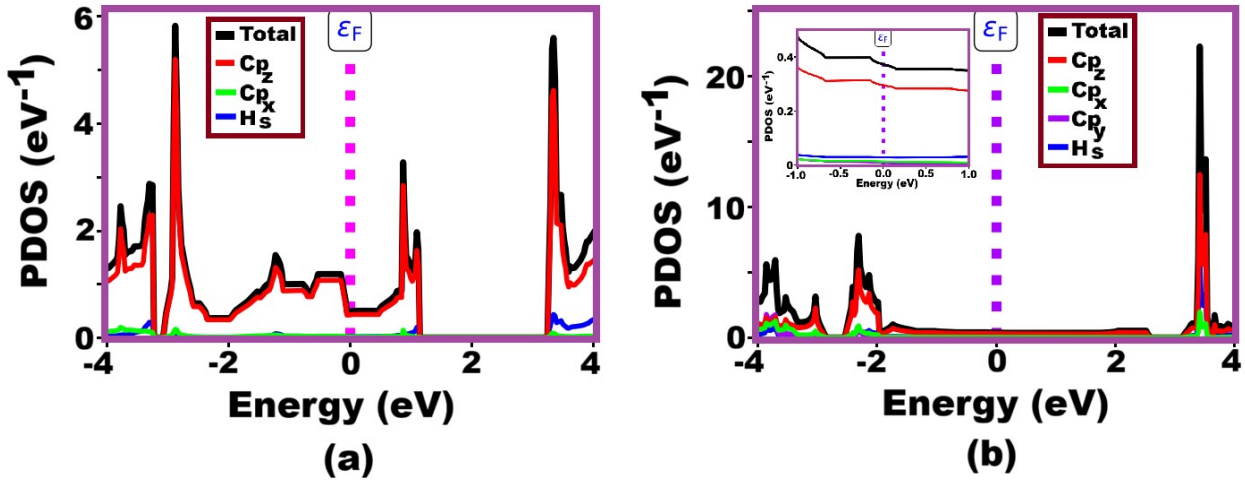

Figure S2. Projected density of states (PDOS) (a) 1H-decorated pentahexoctite and (b) 3H-decorated pentahexoctite.

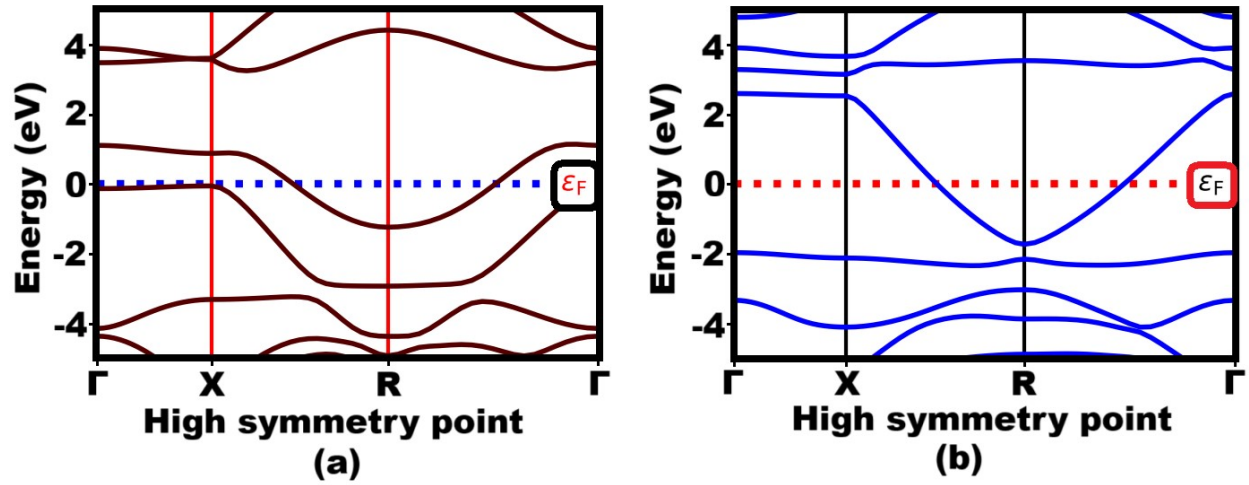

Figure S3: Bandstructure of H-decorated pentahexoctite; (a) 1H-decorated pentahexoctite and (b) 3H-decorated pentahexoctite.

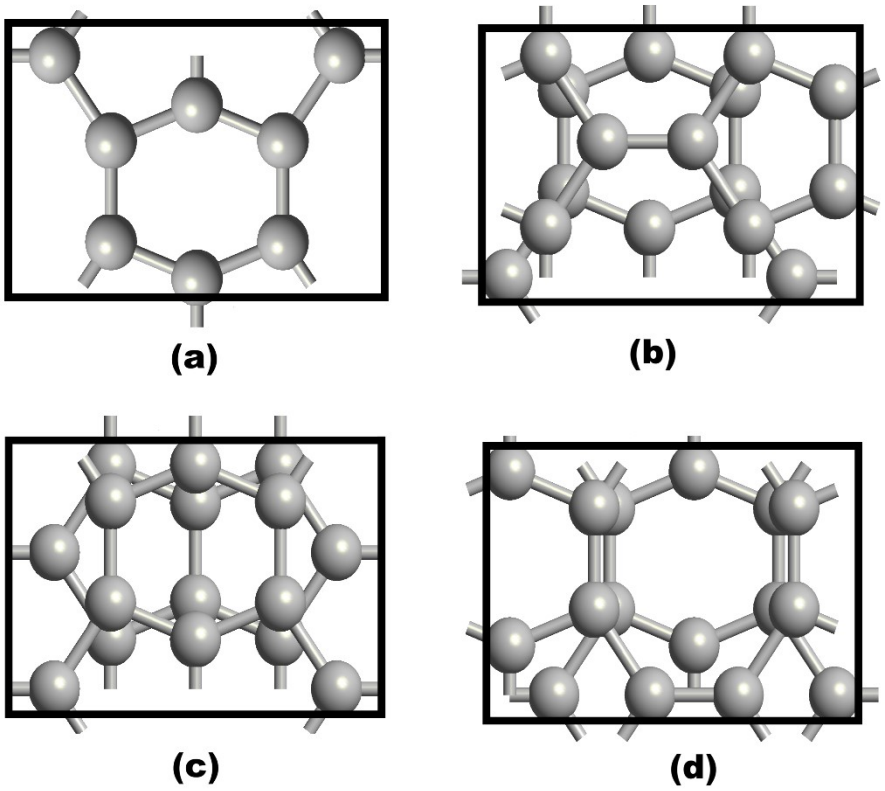

Figure S4: Optimized strucrure of (a) AA stacking mode, (b) AB stacking mode, (c) AC stacking mode and (d) AD stacking mode.

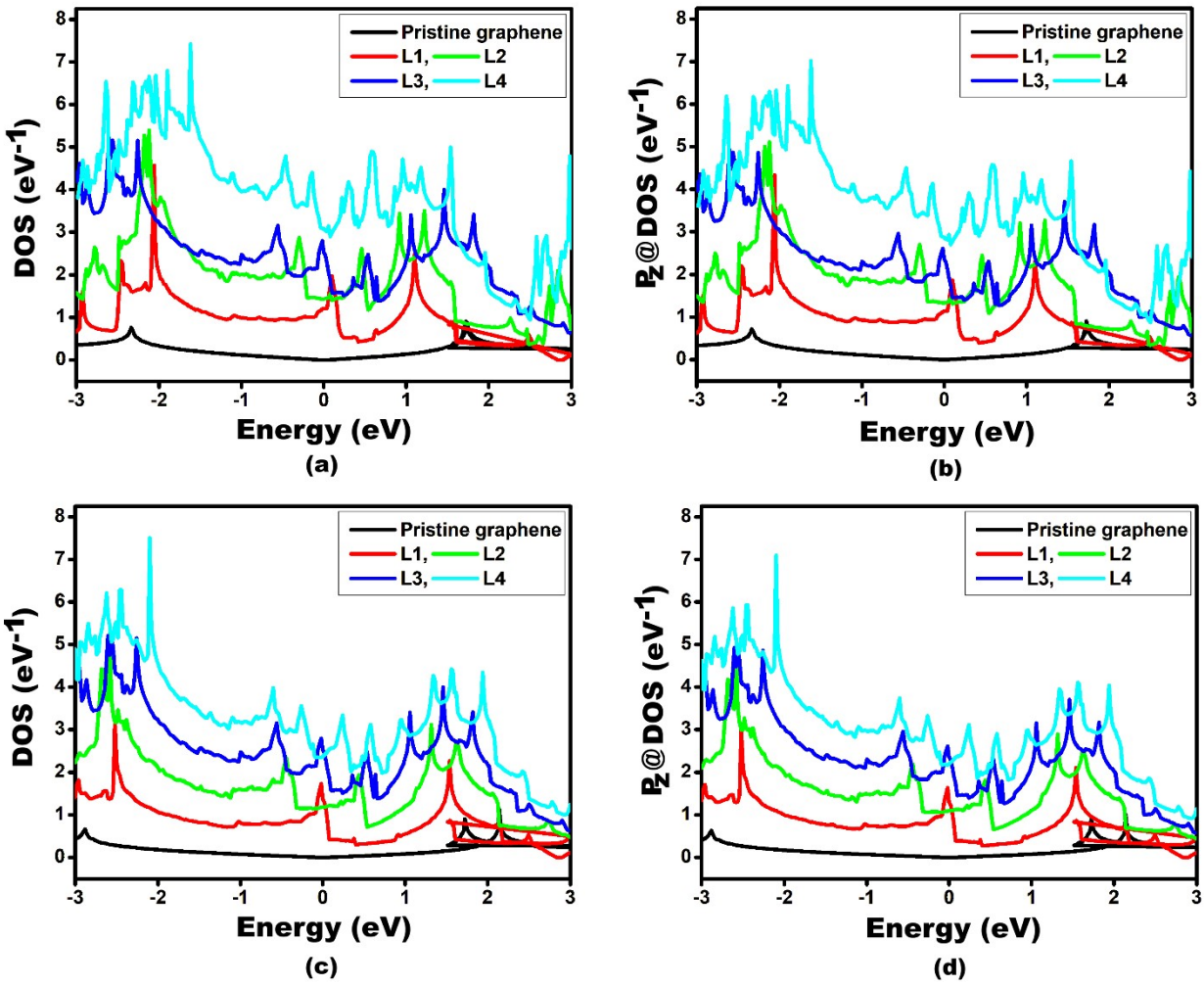

Figure S5: Density of states (a) for PBE-D3 functional (c) for HSE06 functional. Density of states of p_z contribution (b) for PBE-D3 functional and (d) for HSE06 functional for pristine graphene, pentahexoctite and its multi-layers (L1, L2, L3 and L4).

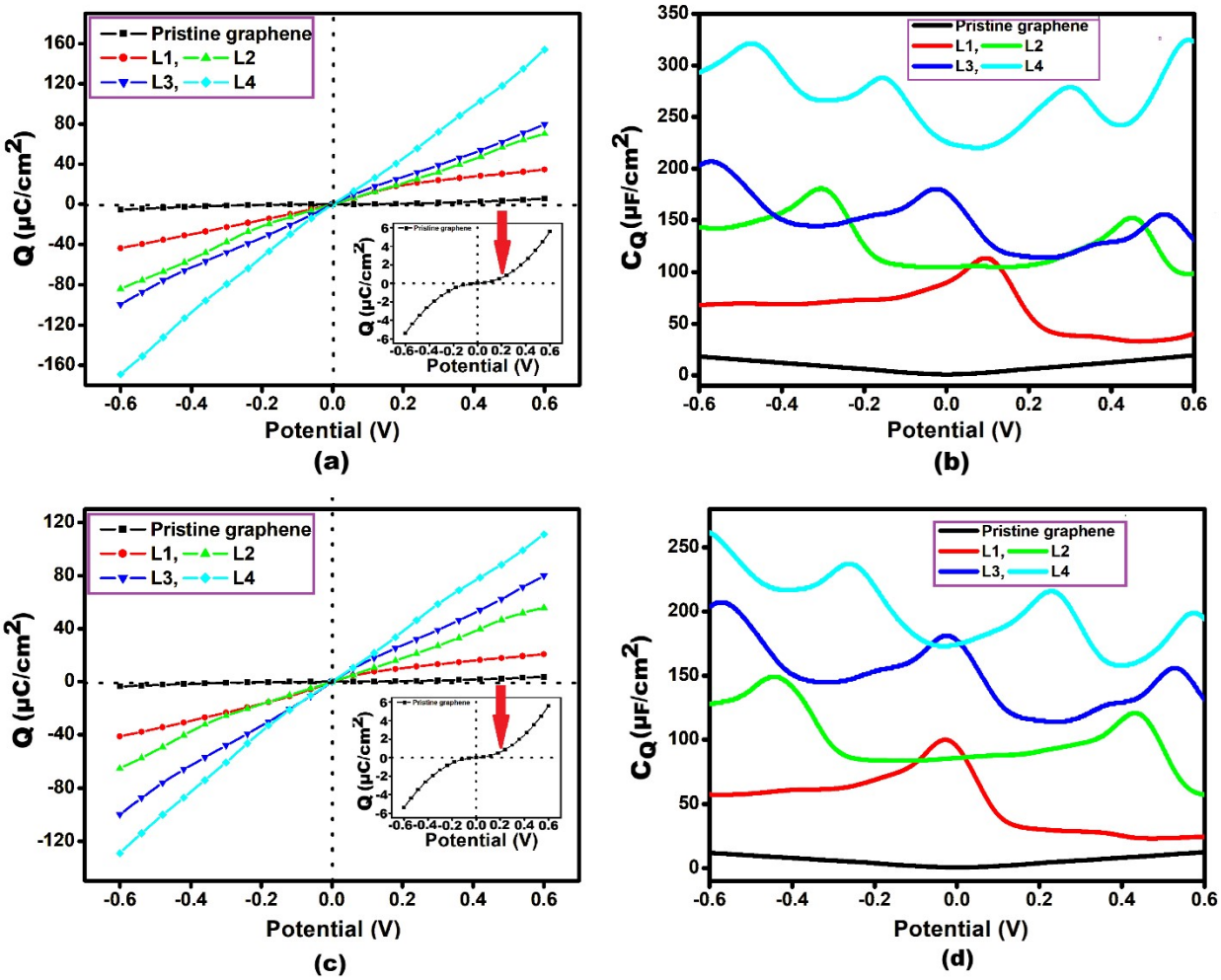

Figure S6: Surface charge density (a) for PBE-D3 functional (c) for HSE06 functional. Quantum capacitance (b) for PBE-D3 functional and (d) for HSE06 functional for pristine graphene, pentahexoctite and its multi-layers (L1, L2, L3 and L4).

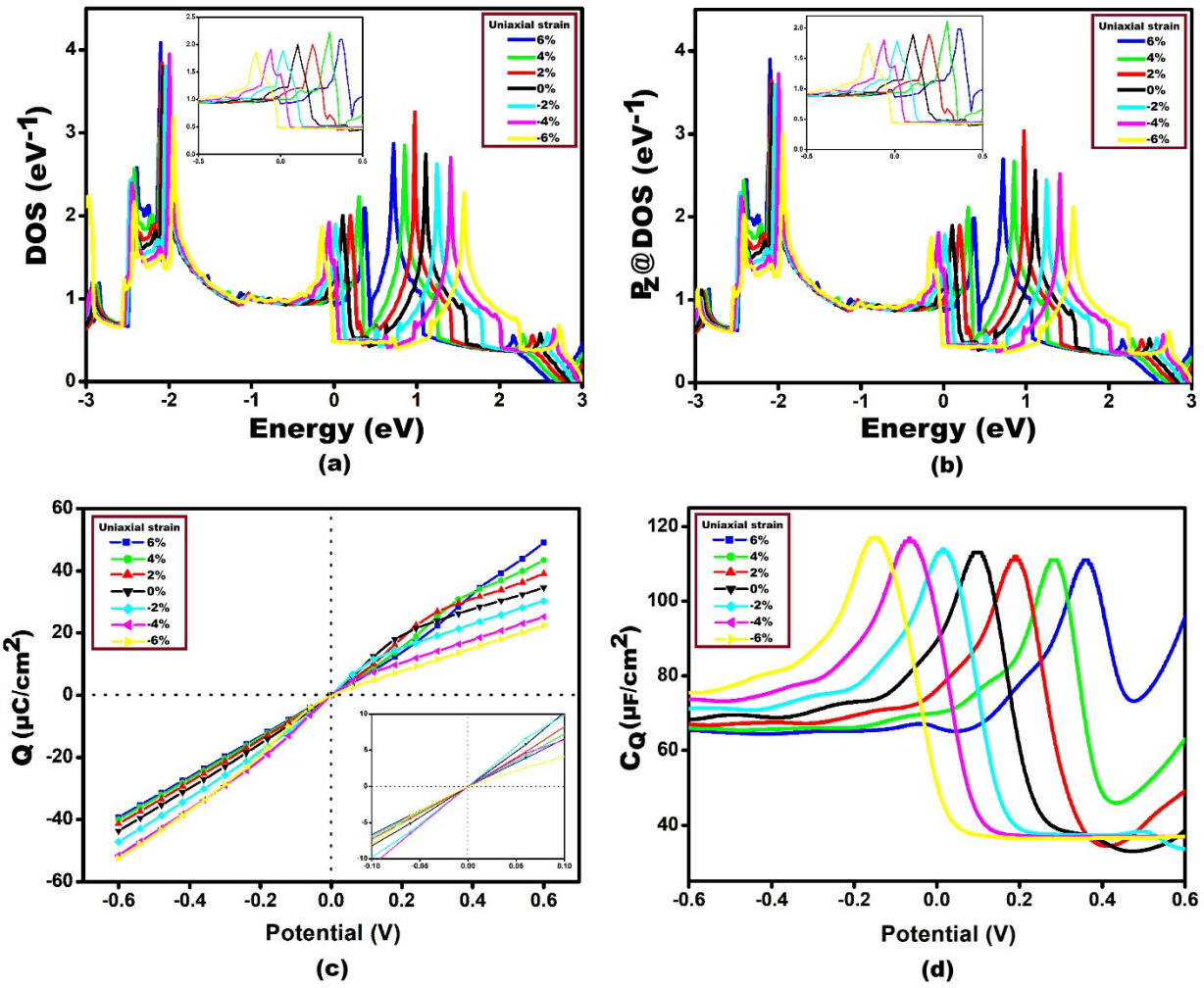

Figure S7: (a) Density of states, (b) density of states of p_z contribution to DOS and (c) Surface charge density and (d) quantum capacitance of pentahexoctite for uniaxial strain.

Table S1: The maximum surface charge density (Q^+ and Q^-) and nature of electrode type of multi-layered pentahexoctite using PBE-D3 and HSE06 functional.

Effect of multi-layered structure (PBE-D3 functional)				
System	**Q^+ (μC/cm²)**	**Q^- (μC/cm²)**	**$\|Q^+/Q^-\|$**	**Electrode type**
L1	34.479	-43.677	0.789	Negative
L2	70.213	-83.794	0.837	Negative
L3	79.657	-99.375	0.802	Negative
L4	153.939	-168.684	0.913	Symmetric

Effect of multi-layered structure (HSE06 functional)				
L1	20.623	-41.212	0.500	Negative
L2	55.664	-65.151	0.854	Negative
L3	79.950	-99.740	0.801	Negative
L4	110.801	-129.446	0.856	Negative