

# ***Ab initio* calculation of ionization potential and electron affinity in solid-state organic semiconductors**

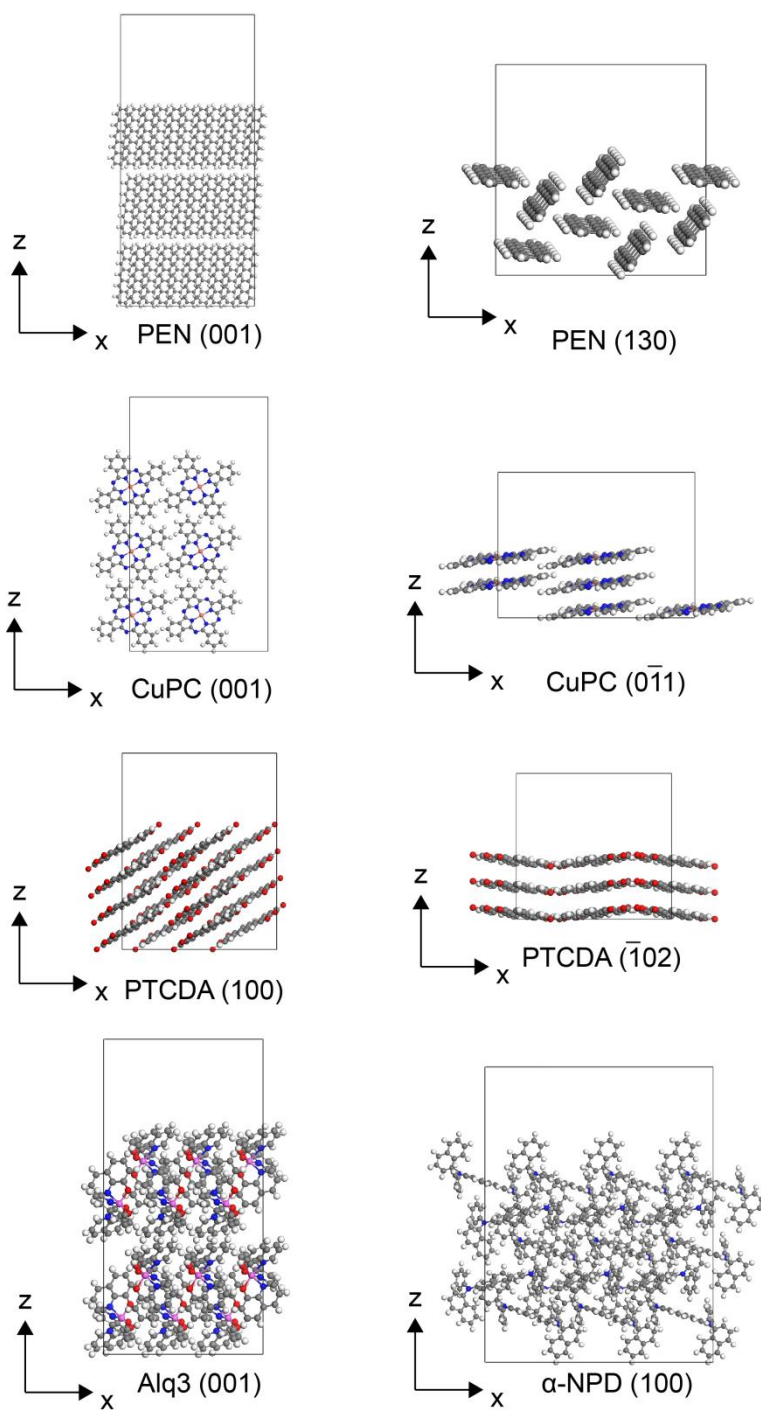
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**- Supplement Information -**

## 1. Molecular geometries adopted in this study for slab calculation



**Figure S1.** The supercell with adopted surface orientation for the slab calculation.