

Supporting Information

**With the Same Clar Formulas, Do the Two-dimensional Sandwich
Nanostructures X-Cr-X (X=C₄H, NC₃ and BC₃) Behave Similarly?**

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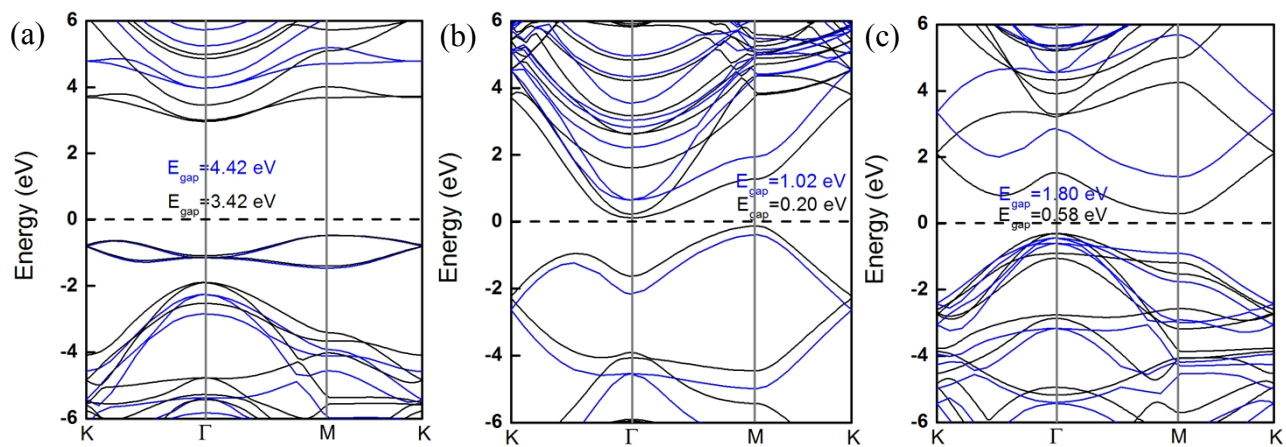
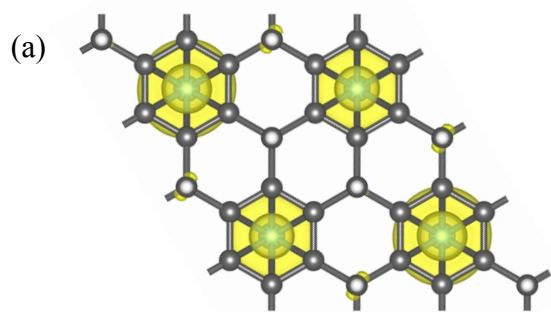
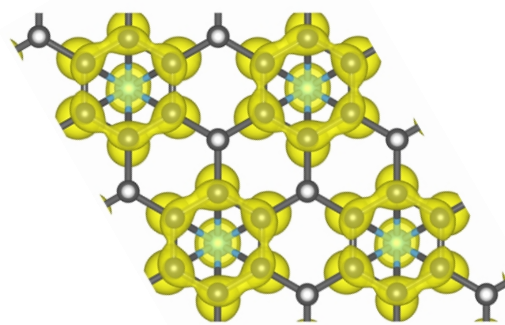


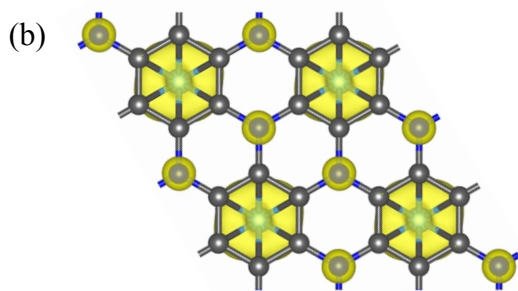
Figure S1: Calculated electronic band structure of isolated 2D (a) C_4H , (b) NC_3 and (c) BC_3 monolayers using PBE (black lines) and hybrid HSE06 (blue lines) functionals.



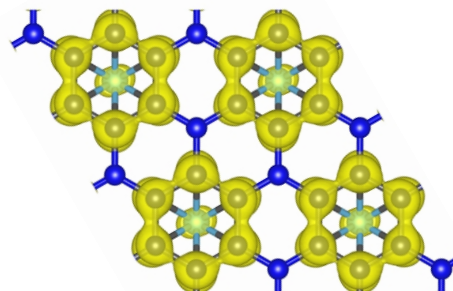
$C_4H-Cr-C_4H$ in AA stacking-H1 (VBM)



$C_4H-Cr-Cr-C_4H$ in AA stacking-H1 (CBM)



$NC_3-Cr-NC_3$ in AA stacking-H1 (VBM)



$NC_3-Cr-NC_3$ in AA stacking-H1 (CBM)

Figure S2: The electron density isosurfaces for VBM and CBM of the NM phase of AA stacking-H1 (a) $C_4H-Cr-C_4H$ and (b) $NC_3-Cr-NC_3$. The isovalue is 0.001 au.