

Supplementary information for

**C₅₄Si₆ heterofullerene as potential gas sensors for CO, NO, and HCN
detection**

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1. The configurations, adsorption energies and adsorption distances of the CO, NO, and HCN molecules adsorbed on $C_{54}Si_6$ heterofullerene with considering van der Waals interaction.

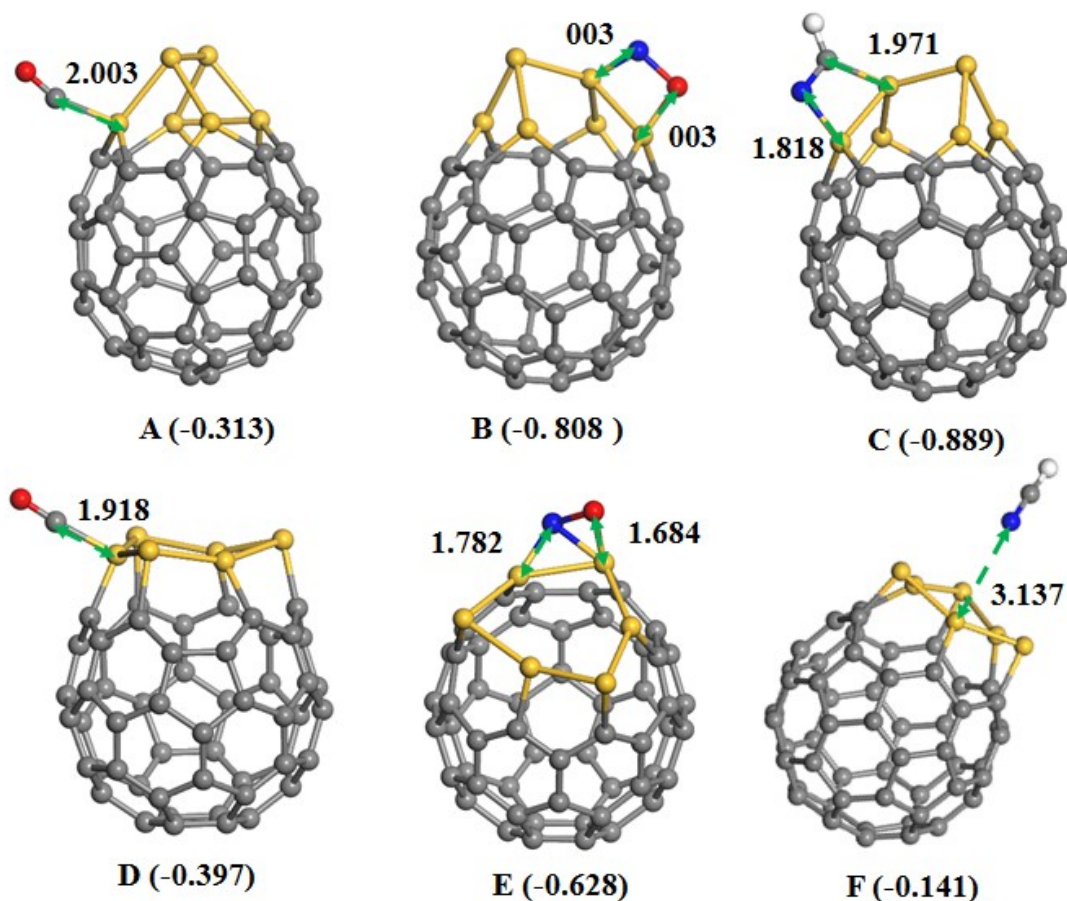


Fig. S1. The most stable configurations of $C_{54}Si_6$ heterofullerene with the gas molecule adsorption: (A) CO, (B) NO, (C) HCN adsorbed on the isomer-1 of $C_{54}Si_6$, (D) CO, (E) NO, (F) HCN adsorbed on the isomer-2 of $C_{54}Si_6$. Values in parentheses are adsorption energies in eV. Bond distances are in angstrom. These results are obtained by using the dispersion-corrected DFT (DFT-D) based on Tkatchenko–Scheffler methods.