

Supplementary information

Geometrical structure and electronic properties of Ni-cCN and Ni-pGN

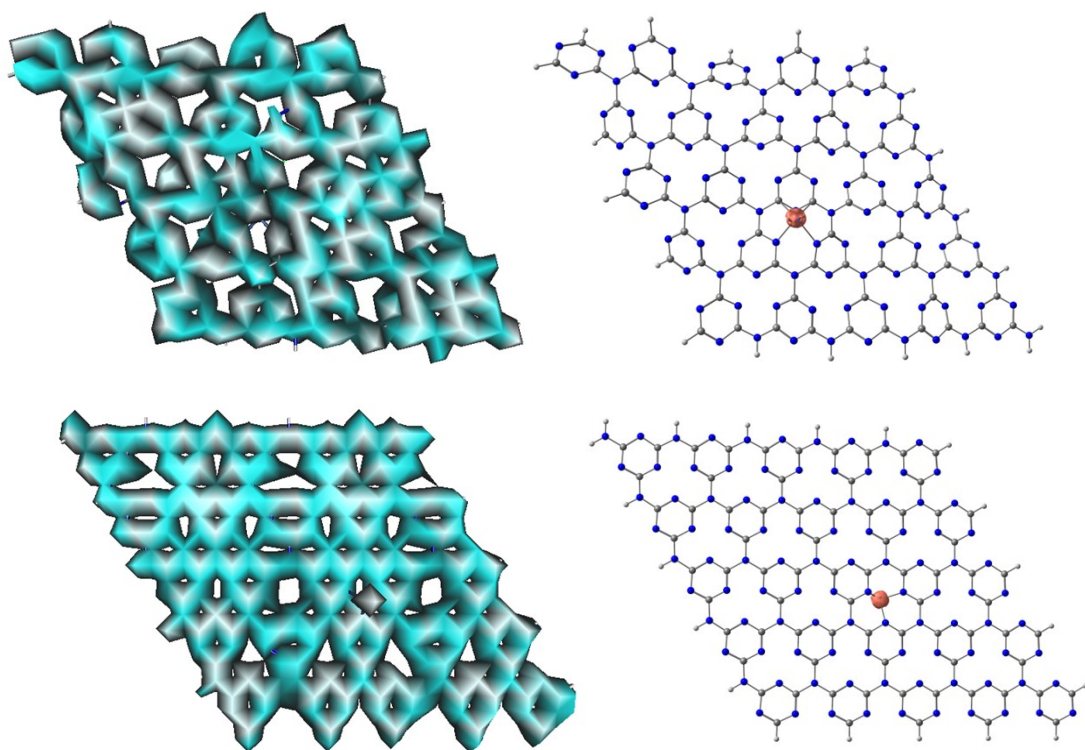


Figure 1. Electron density of Ni-gCN depicted at an isovalue of $0.03 \text{ e}/\text{\AA}^3$ and FOD of Ni-gCN depicted at an isovalue of $0.01 \text{ e}/\text{\AA}^3$: a) – Ni-cGN, b) – Ni-pGN

Interaction between HCH and Ni-cGN and Ni-pGN

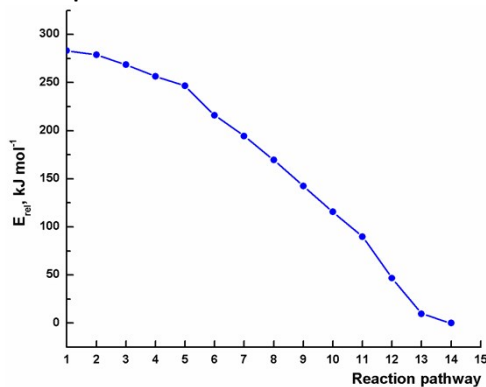


Figure 2. Relative energies (E_{rel}) of the configurations that occur during the adsorption of HCH on Ni-cGN system, $E_{\text{final}} = 0.00 \text{ kJ mol}^{-1}$.

The energy of the final product is assumed to be 0.00 kJ mol^{-1} .