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"Supplementary Materials"

Synergic effects between boron and nitrogen atoms in BN-codoped $C_{59-n}BN_n$ fullerenes (n=1-3) for metal-free reduction of greenhouse N_2O gas

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Figure S1. The relaxed structures of single-vacancy defective fullerenes (from top and side views)

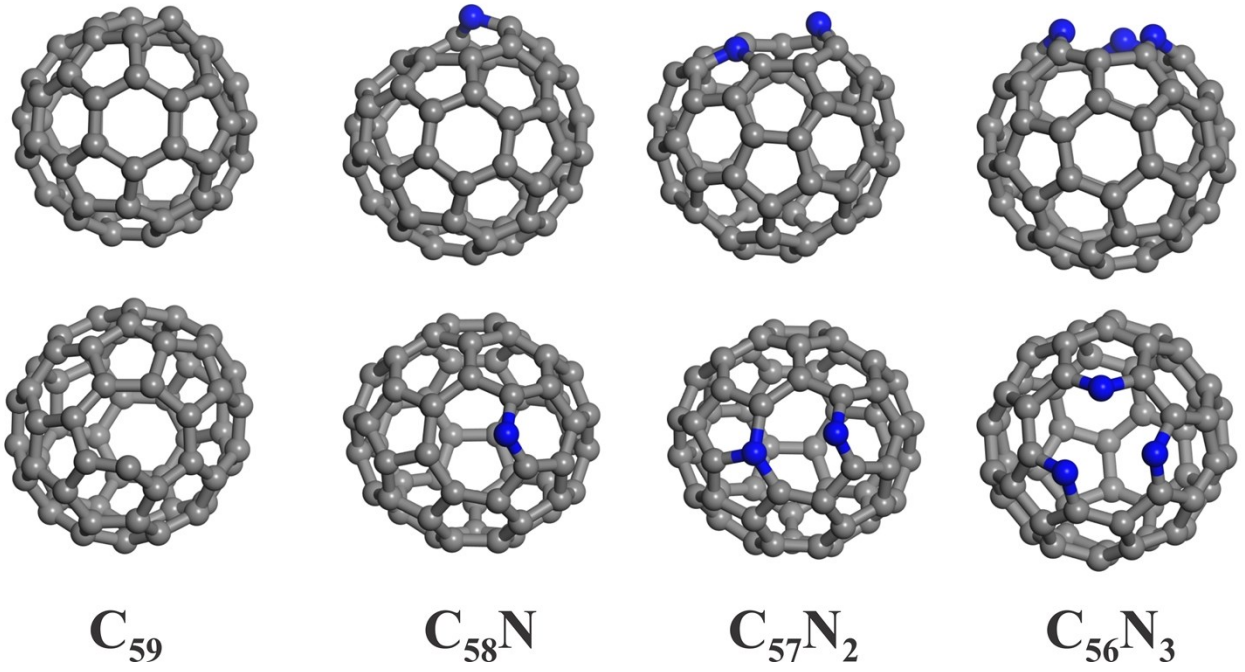

Figure S2. The geometries of BN-codoped fullerenes after the MD simulations (2000 fs, at 600 K) and the corresponding energy profile

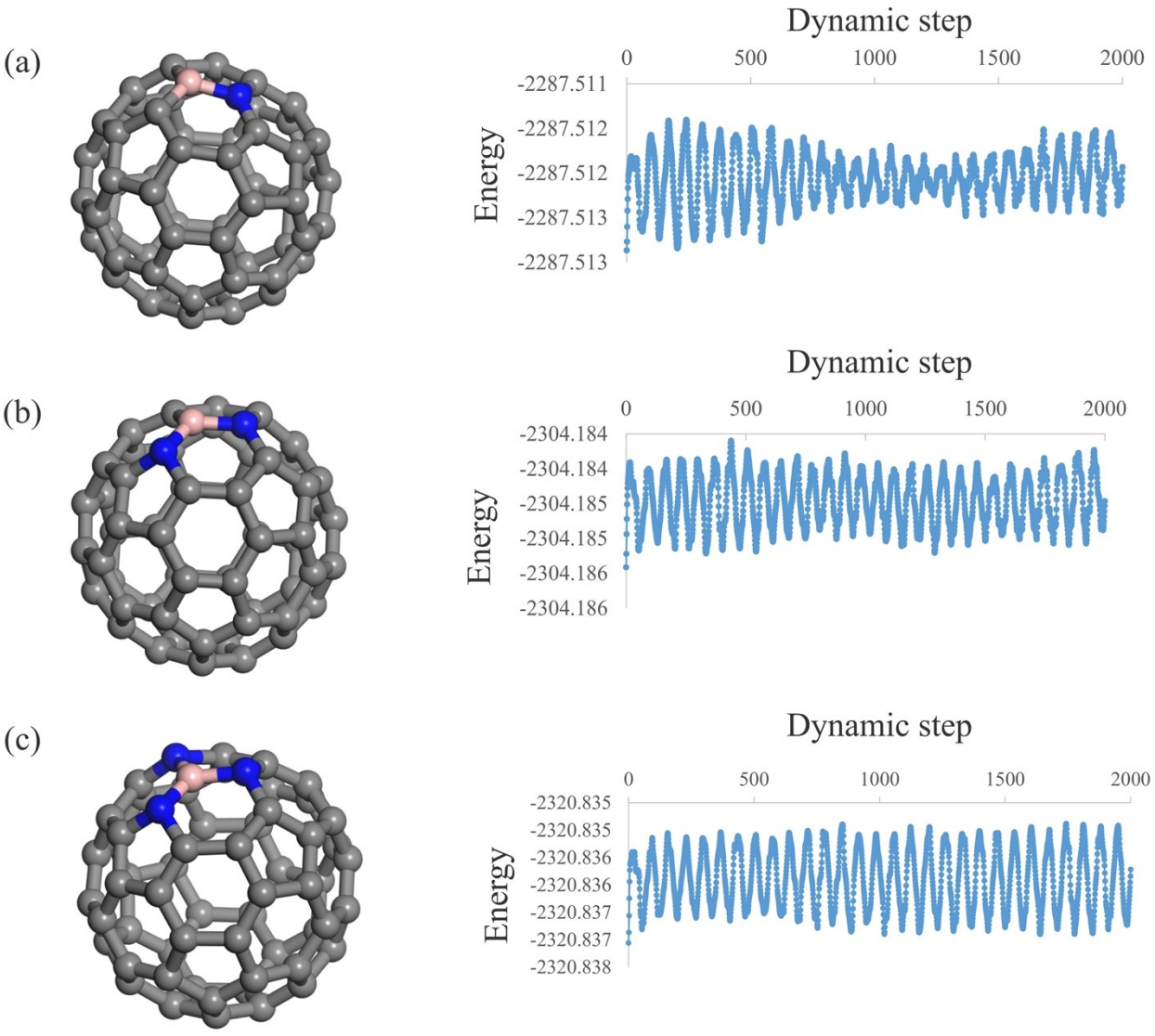

Figure S3. The relaxed structures of N_2O (left) and CO adsorbed (right) configurations onto Kr endohedral fullerenes (a) $C_{59}B$, (b) $C_{58}BN$, (c) $C_{57}BN_2$ and (d) $C_{56}BN_3$