Electronic Supplementary Material (ESI) for New Journal of Chemistry.

“Supplementary Materials”

Efficient hydrogen storage on Al decorated $C_{24}N_{24}$: A DFT study

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Figure S1. The geometries of $AlC_{24}N_{24}$ after the AIMD simulations at 600 and 1000 K (2000 fs)

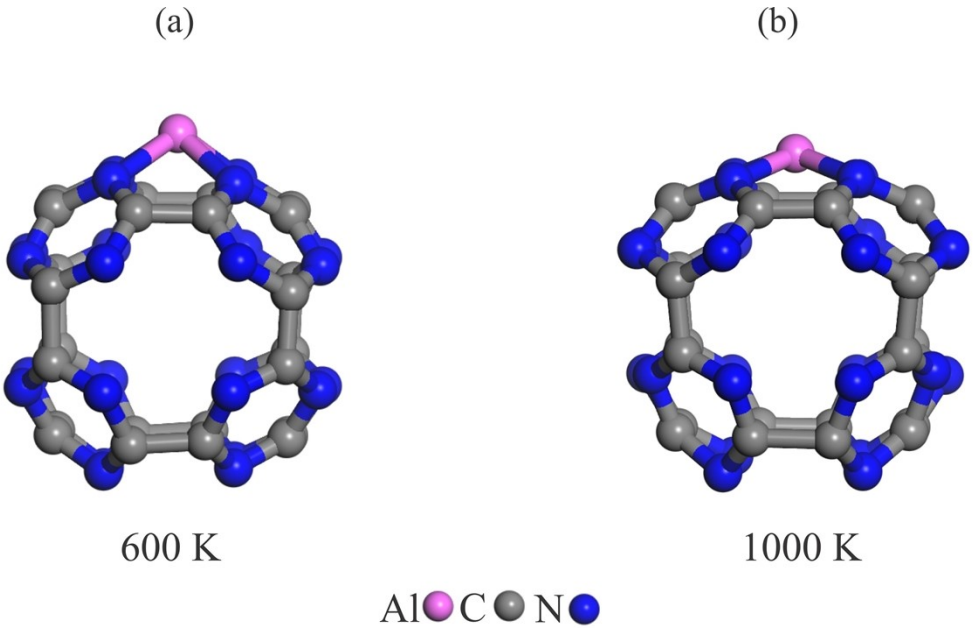

Figure S2. The geometries of $Al_6C_{24}N_{24}$ after the AIMD simulations at 600 and 1000 K (2000 fs)

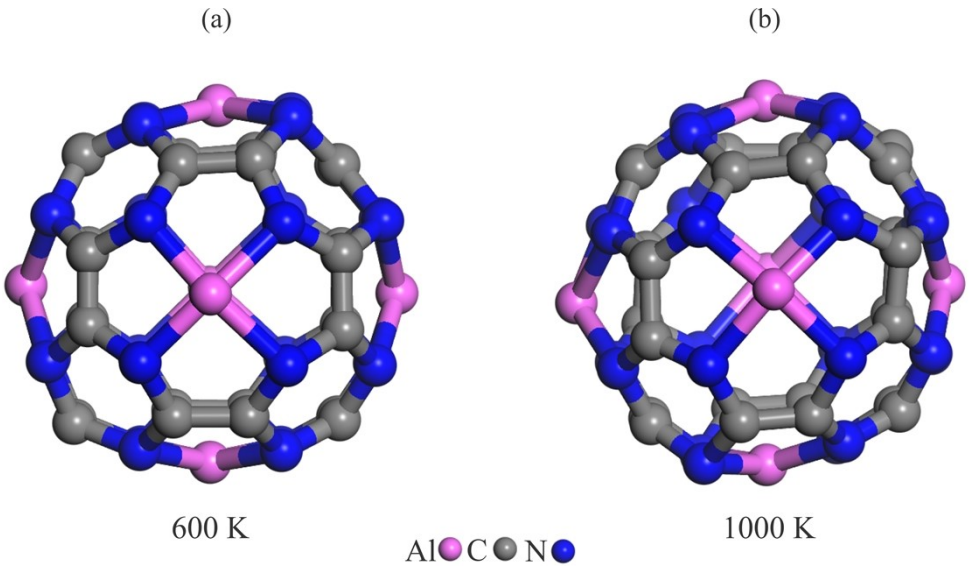

Figure S3. Molecular graphs of $AlC_{24}N_{24}:H_2$ (configuration **A**) (a), $AlC_{24}N_{24}:H_2$ (configuration **B**) (b), $AlC_{24}N_{24}:(H_2)_2$ (c), $AlC_{24}N_{24}:(H_2)_3$ (d), $AlC_{24}N_{24}:(H_2)_2$ (e) and $AlC_{24}N_{24}:(H_2)_2$ (f). The small red circles indicate the BCPs.