Electronic Supplementary Information

Graphene-like Mg_3N_2 Monolayer: High Stability, Desirable Direct Band Gap and Promising Carrier Mobility

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SUPPORTING INFORMATION

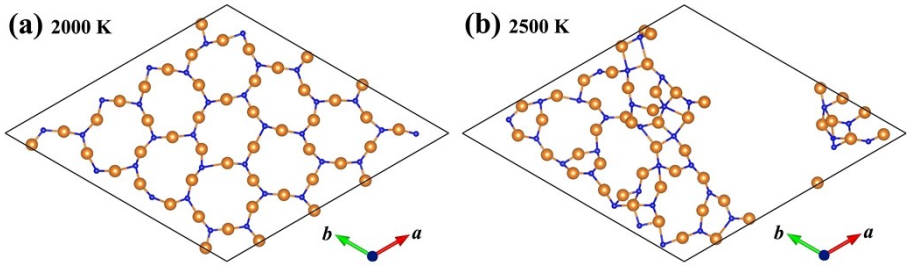

Figure S1. Top view of a snapshot of monolayer g-Mg_3N_2 of the *ab-initio* molecular dynamics simulation at (a) 2000 K and (b) 2500 K. 4 × 4 × 1 supercell is used and labeled by black solid line.

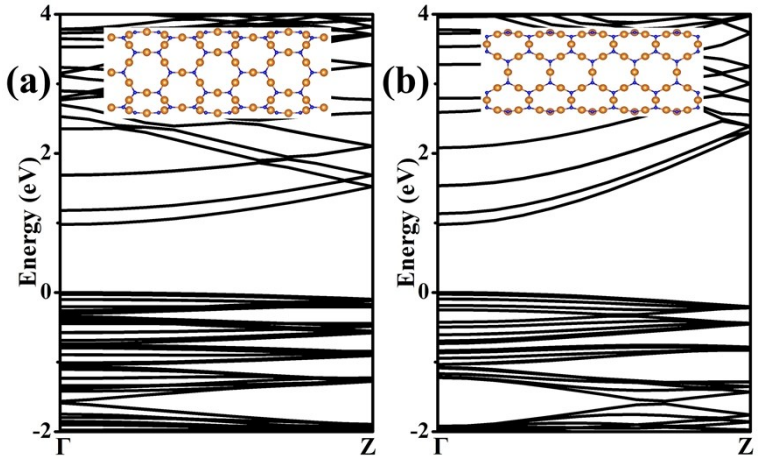

Figure S2. Band structure of armchair (6,6) and zigzag (8,4) tubes.

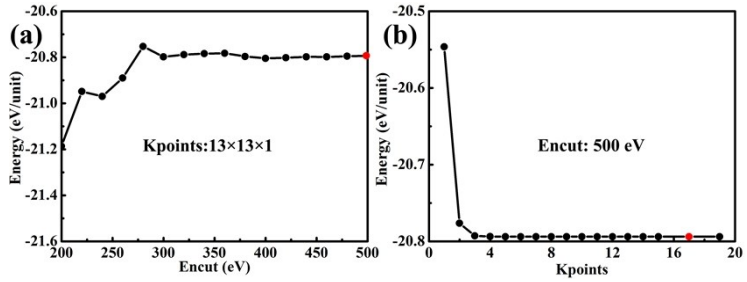

Figure S3. The convergence tests for (a) K-point grids and (b) cutoff energy. Red dots are the parameters we have used in the calculations.

Table S1. The calculated energies of 2D g-Mg_3N_2, isolated Mg and isolated N atoms, respectively.

System	g-Mg_3N_2	isolated Mg atom	isolated N atom
Energy (eV)	–20.764	–0.075	–3.124