Supporting Information

Potential Hydrogen Storage Materials from Metal Decorated 2D-C_2N: An Ab-initio Study

R. Varunaa,[1,2] and P. Ravindran[1,2,3,*]
[1]Department of Physics, Central University of Tamil Nadu,
Thiruvarur, 610005, India
[2]Simulation Centre for Atomic and Nanoscale MATerials (SCANMAT),
Central University of Tamil Nadu, Thiruvarur, 610005, India
[3]Center for Materials Science and Nanotechnology and Department of Chemistry,
University of Oslo, Box 1033 Blindern, N-0315 Oslo, Norway
E-mail: raviphy@cutn.ac.in

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Table S1: Calculated binding energy for seven possible adsorption sites of H_2 molecule in 2D-C_2N.

H_2 position in 2D-C_2N	Binding energy (eV/H_2)
Top of C (TC)	0.052
Top of N (TN)	0.058
C-C bridge site (BCC)	0.042
C-N bridge site (BCN)	0.056
Hollow site of C−C ring (HCC)	0.043
Hollow site of C−N ring (HCN)	0.048
Center of holey site (P)	0.099

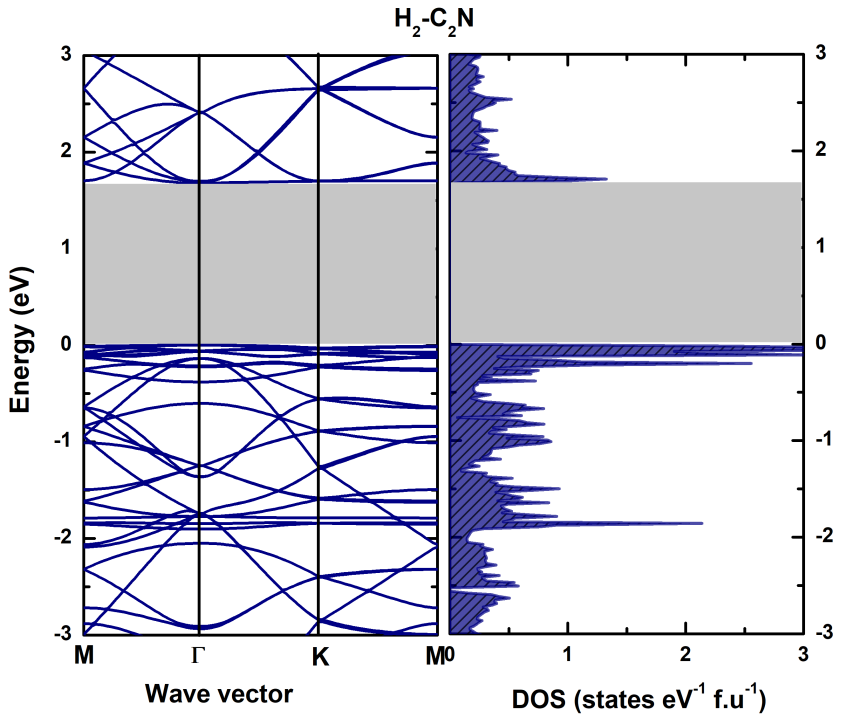

Figure S1: Calculated band structure and total DOS of H_2-C_2N using PBE functional.

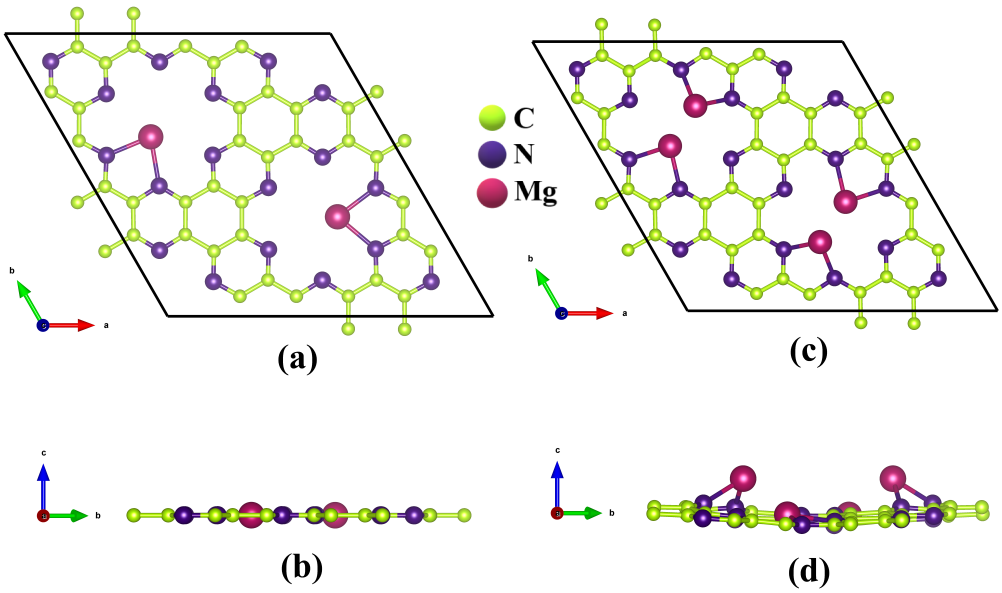

Figure S2: (a) and (c) Top view, (b) and (d) side view of the optimized structure of Mg_2C_2N and Mg_4C_2N @ 0 K, respectively.

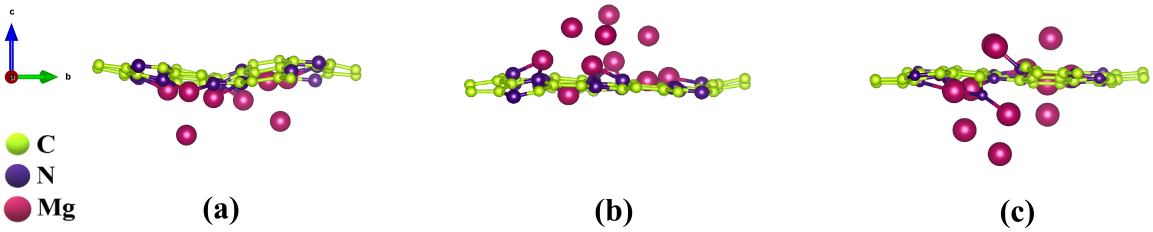

Figure S3: The side view of the optimized structure of (a) Mg_8C_2N, (b) $Mg_{10}C_2N$, and (c) $Mg_{12}C_2N$ @ 300 K.

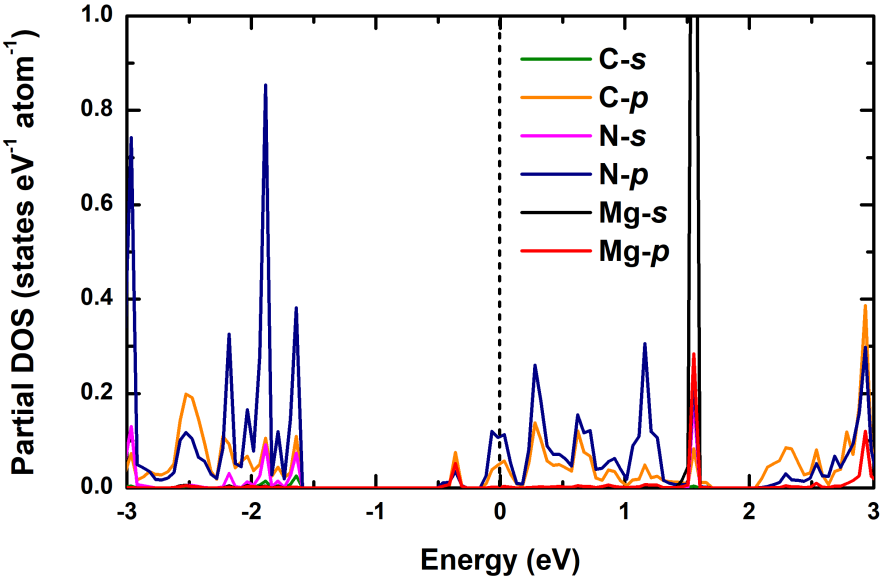

Figure S4: Calculated partial DOS of Mg_2C_2N using PBE functional.

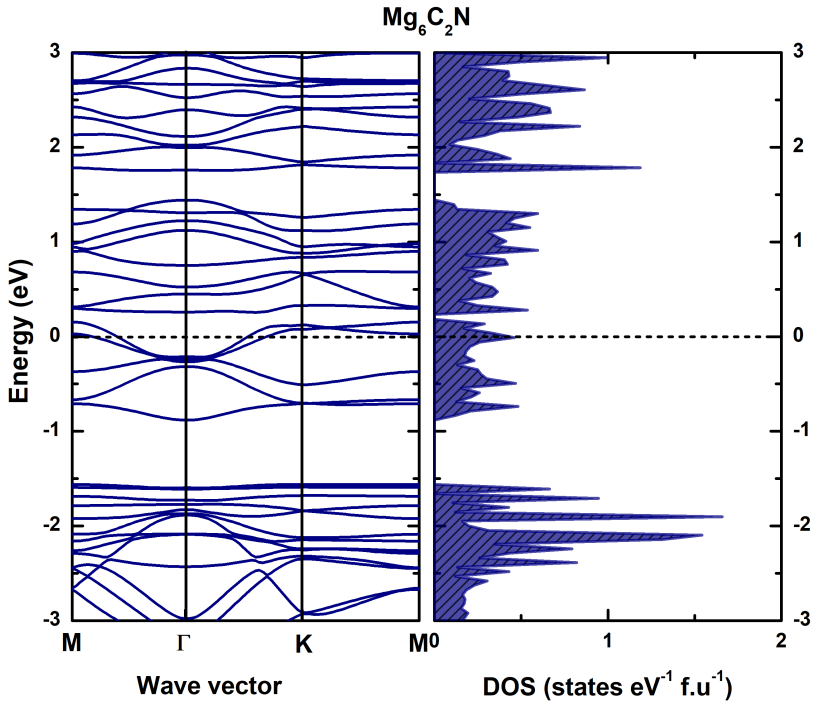

Figure S5: Calculated band structure and total DOS of Mg_6C_2N using PBE functional.

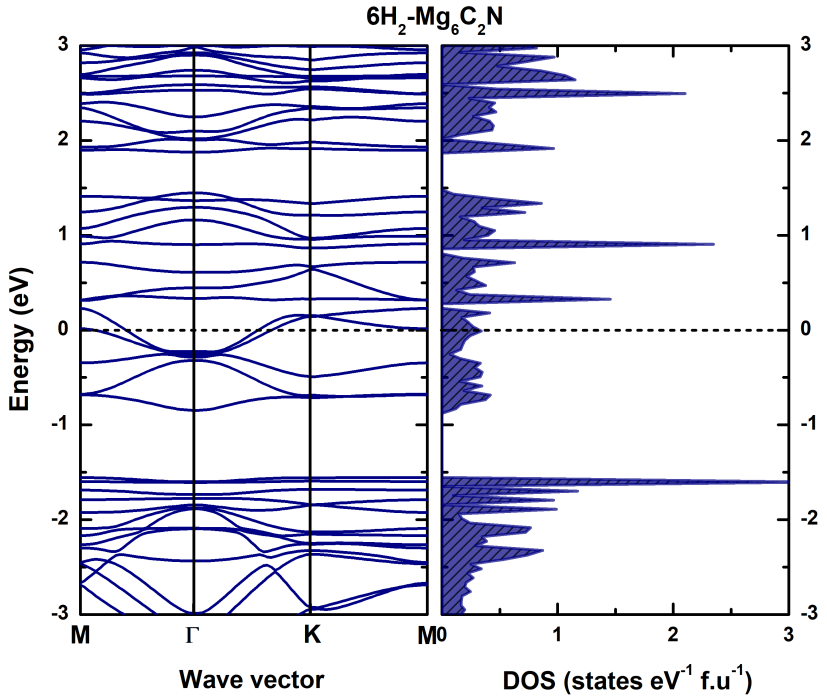

Figure S6: Calculated band structure and total DOS of $6H_2$-Mg_6C_2N using PBE functional.

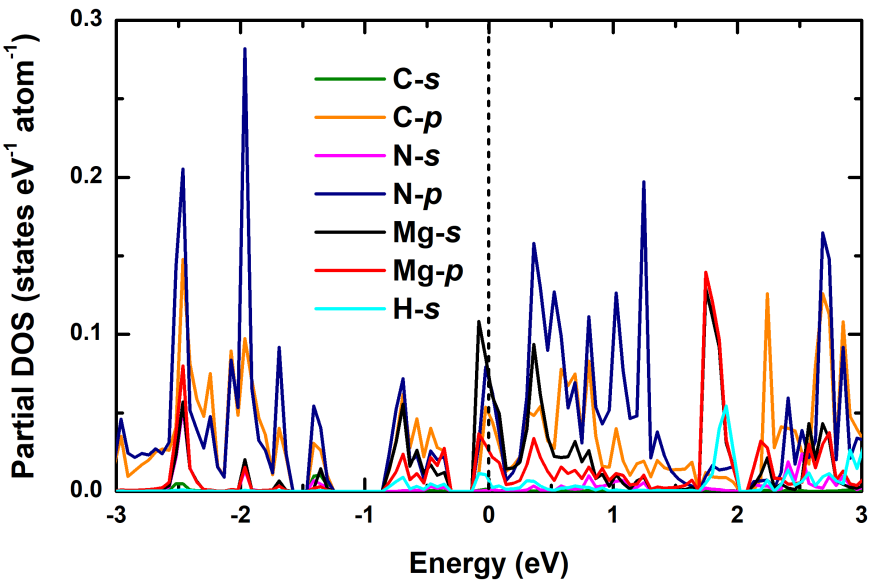

Figure S7: Calculated partial DOS of $30H_2$-Mg_6C_2N using PBE functional.