Supporting Information for

First principles study of *g*-Mg_3N_2 as anode material for Na-, K-, Mg-, Ca- and Al-ion storage

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SI-1. Adsorption energies of metal-ions

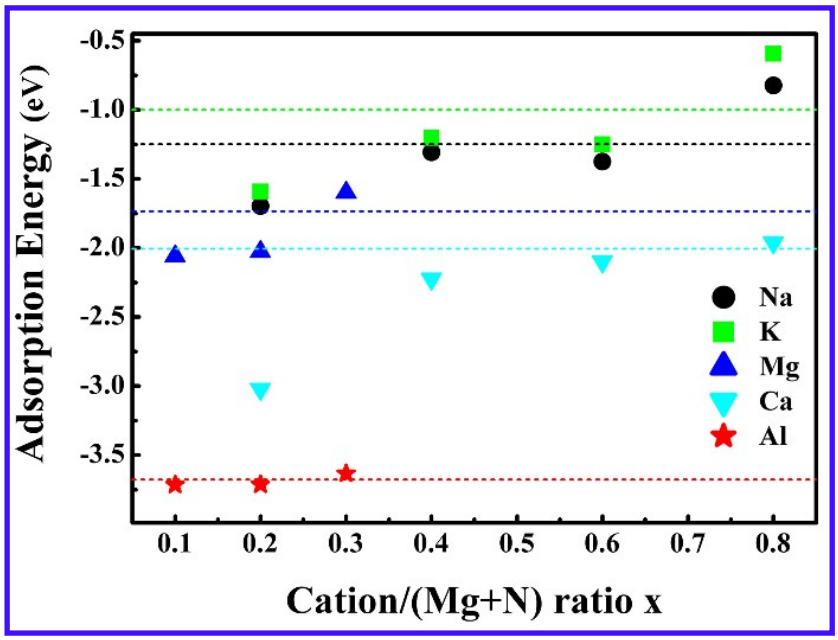

Fig. S1. Calculated sequential metal-ion adsorption energies on *g*-Mg_3N_2 as a function of the adsorption concentration *x*. The dotted lines represent the cohesive energies of the corresponding bulk phase metals.

SI-2. Phonon dispersion data

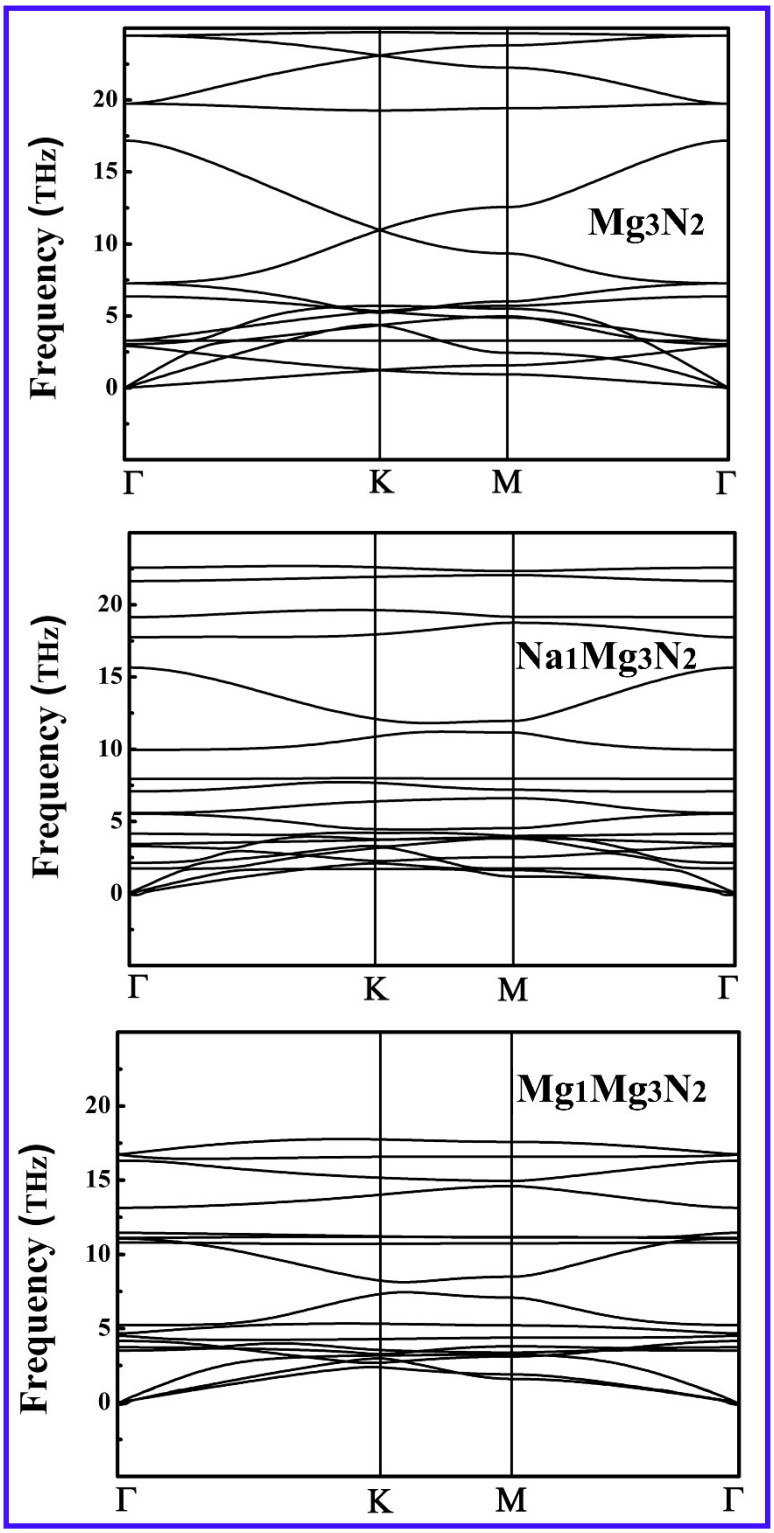

Fig. S2. The phonon dispersion spectrum of *g*-Mg_3N_2, $Na_1Mg_3N_2$ and $Mg_1Mg_3N_2$.

SI-3. Ab-initio molecular dynamics simulation

In order to investigate the thermal stability of *g*-Mg_3N_2 monolayer after metal-ions adsorption, *ab initio* molecular dynamics (AIMD) simulations are performed to check the structural change of the *g*-Mg_3N_2 monolayer at some highest content of adsorbed adatoms ($Na_3Mg_3N_2$, $Mg_1Mg_3N_2$). The results are given in Fig. S1. As is seen, the structure of the *g*-Mg_3N_2 monolayer is changed slightly at 300 K up to 6 ps. Upon relaxation, the structure after the AIMD simulation will recover to its original state, indicating that the bonding/coordination of the structure is not changed at 300 K. Furthermore, no clustering of the adsorbed metal-ions is observed during the AIMD simulation, suggesting that the *g*-Mg_3N_2 monolayer will maintain good cycling stability.

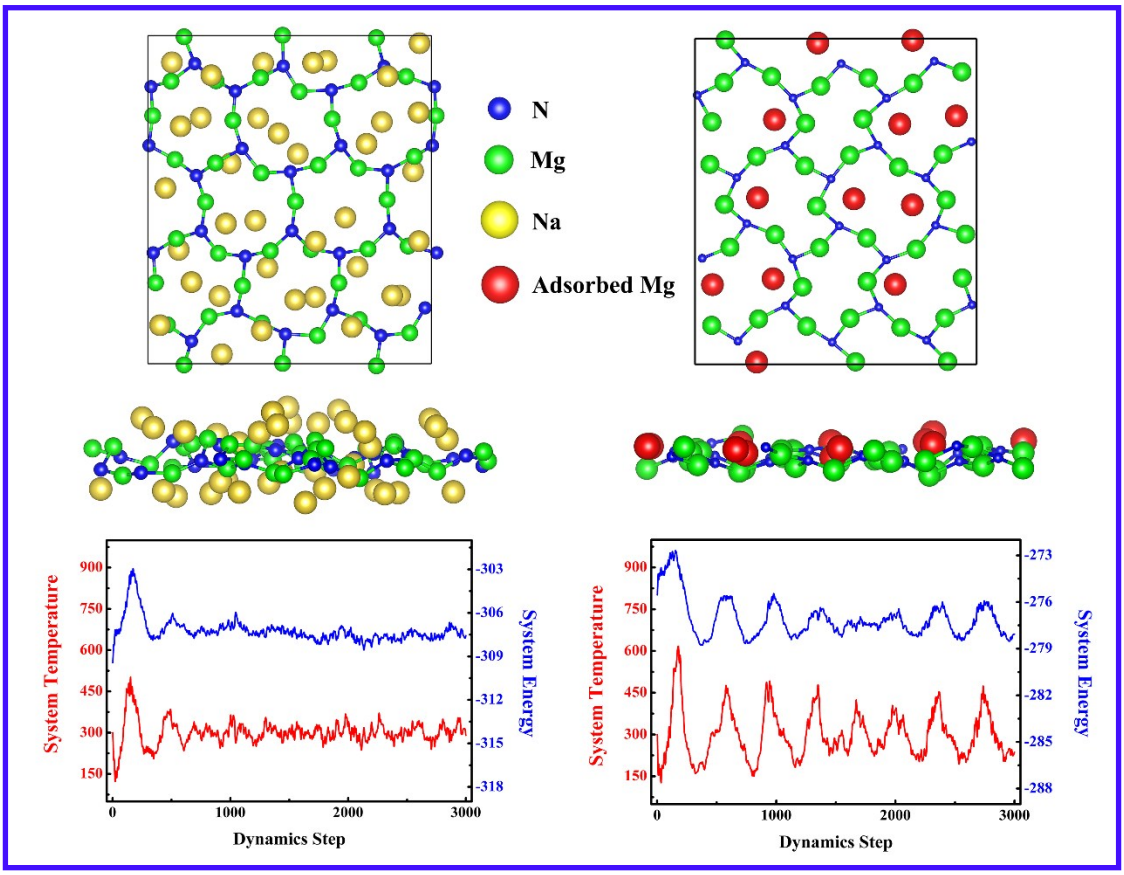

Fig. S3. Top and side views of the structures of *g*-Mg_3N_2 with highest Na- and Mg-ion adsorption concentrations after 6ps of the AIMD simulation at 300 K. The fluctuations of system temperature and energy as functions of simulation time are also presented.