Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

SUPPLEMENTARY MATERIAL

Exfoliation of Borophene from Silver Substrate Assisted by Li/Mg Atoms—A Density Functional Theory Study

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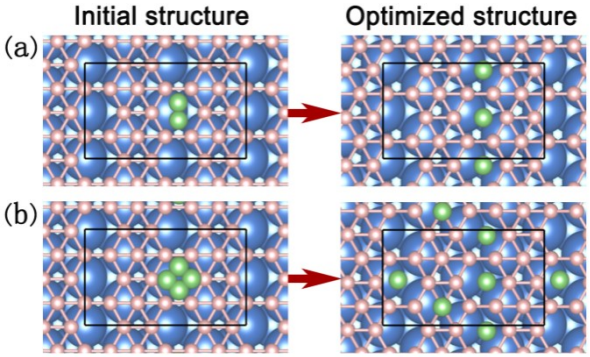

Figure S1. Illustration the optimization of (a) Li_2 and (b) Li_4 clusters on the borophene.

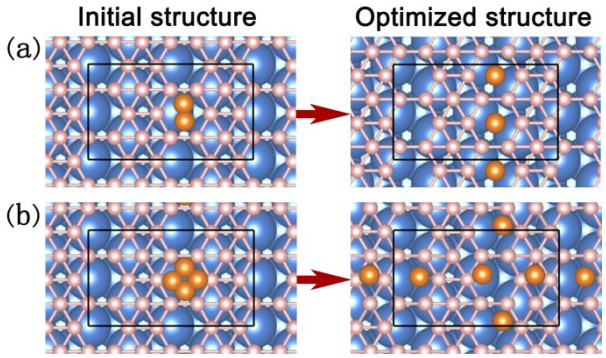

Figure S2. Illustration the optimization of (a) Mg_2 and (b) Mg_4 clusters on the borophene.

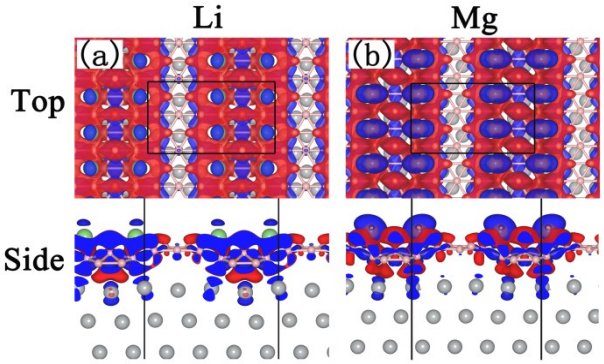

Figure S3. The top and side views of the charge density difference of β_{12} borophene with (a) Li and (b) Mg adatoms. The charge density difference was defined as $\Delta\rho = \rho_{tot} - \rho_{borophene} - \rho_{sub} - \rho_{adatoms}$, where ρ_{tot}, $\rho_{borophene}$, ρ_{sub} and $\rho_{adatoms}$ stand for the charge density of total system, borophene, substrate and Li/Mg adatoms, respectiovely.