

Supporting Information

2D Co-Anti MXenes (CoB/CoP) as Promising Anode Materials for Magnesium-Ion Batteries in Diglyme and Triglyme Electrolytes: A First-Principles Study

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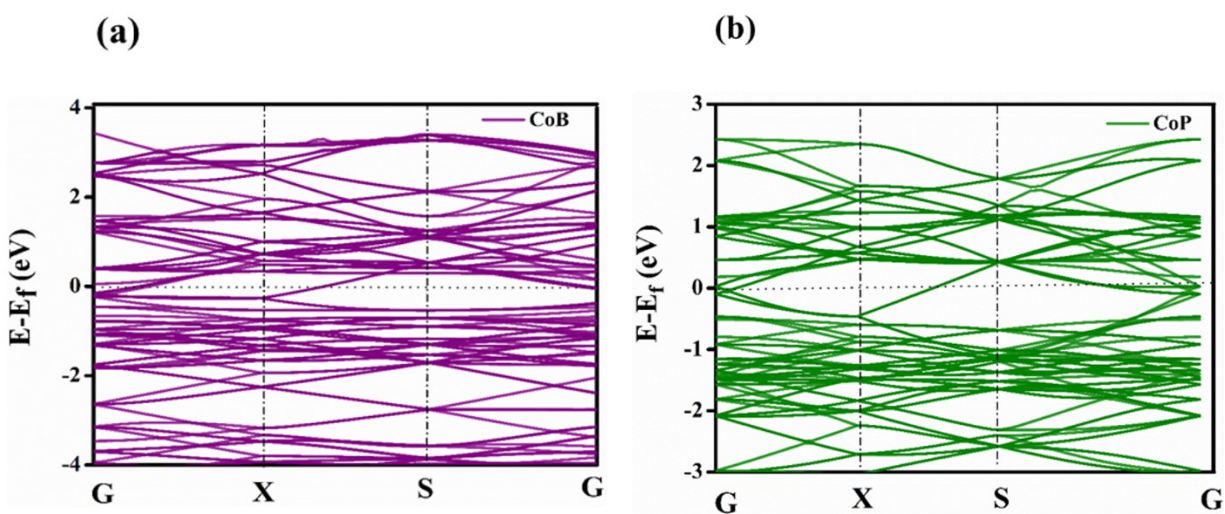
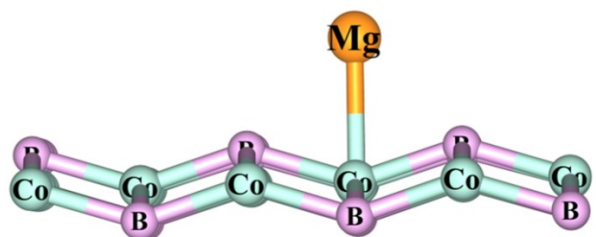
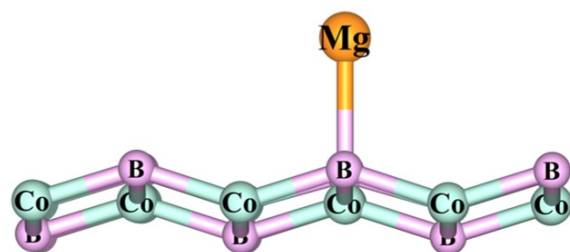


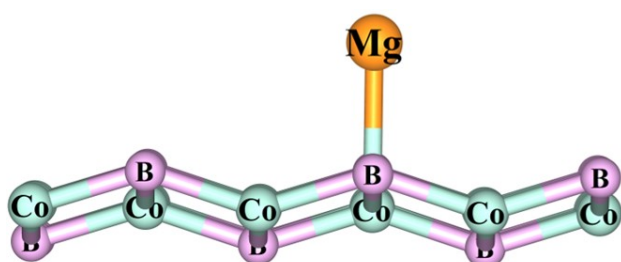
Figure S1. Band structure of (a) CoB and (b) CoP.



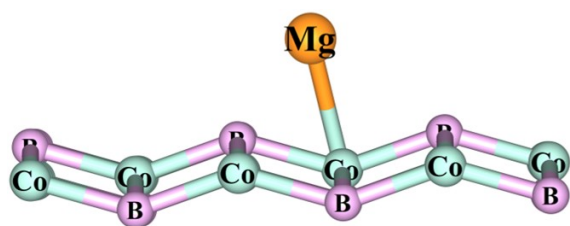
Mg@CoB site 1



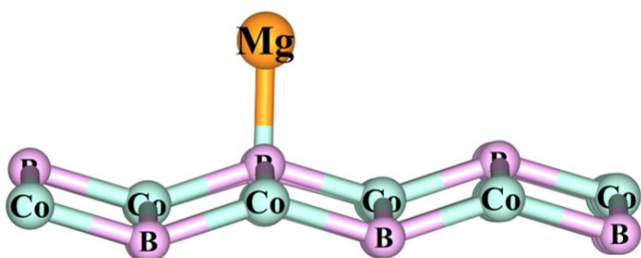
Mg@CoB site 2



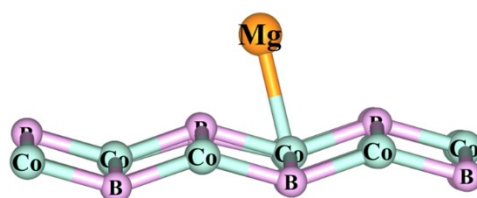
Mg@CoB site 3



Mg@CoB site 4

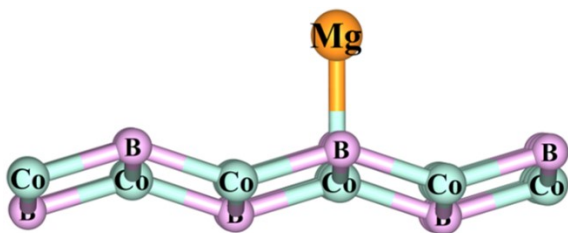


Mg@CoB site 5

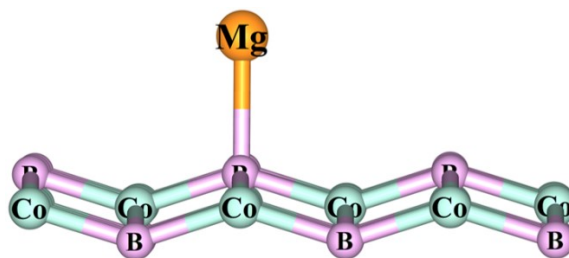


Mg@CoB site 6

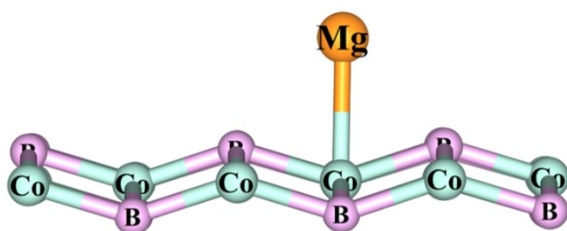
Figure S2. The optimized structure of single Mg atom adsorption on CoB anti-MXene at different sites (diglyme condition).



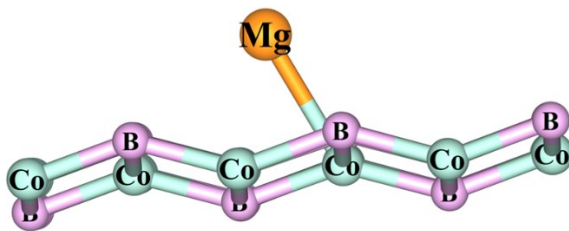
Mg@CoB site 1



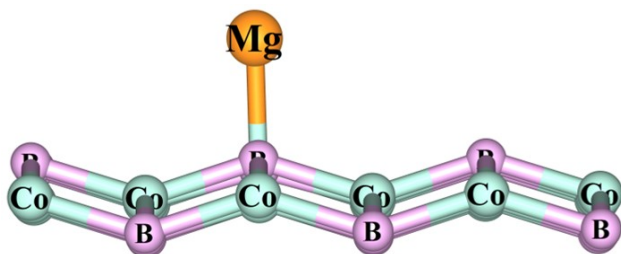
Mg@CoB site 2



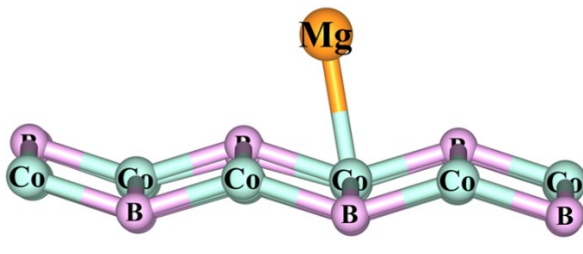
Mg@CoB site 3



Mg@CoB site 4

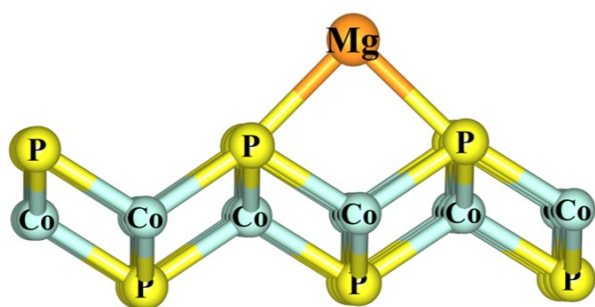


Mg@CoB site 5

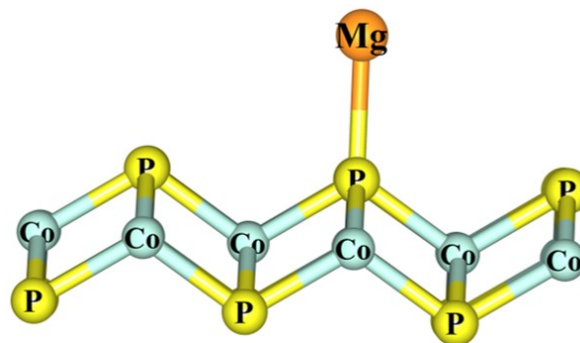


Mg@CoB site 6

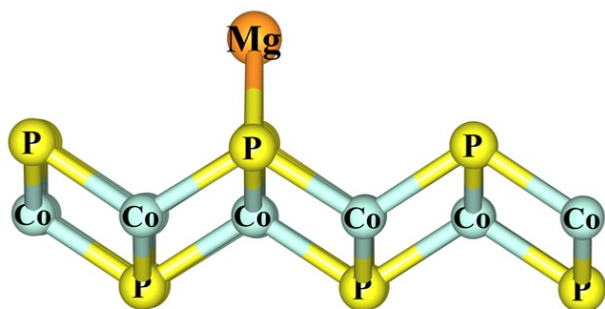
Figure S3. The optimized structure of single Mg atom adsorption on CoB anti-MXene at different sites (triglyme condition).



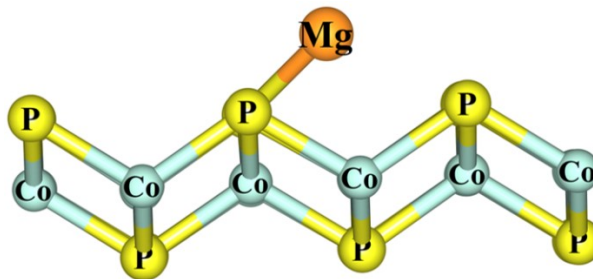
Mg@CoP site 1



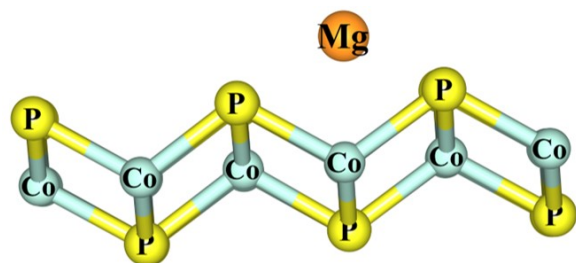
Mg@CoP site 2



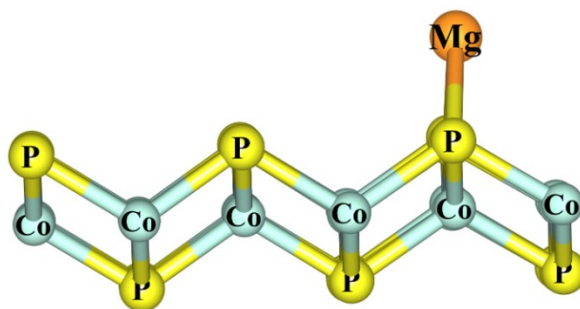
Mg@CoP site 3



Mg@CoP site 4

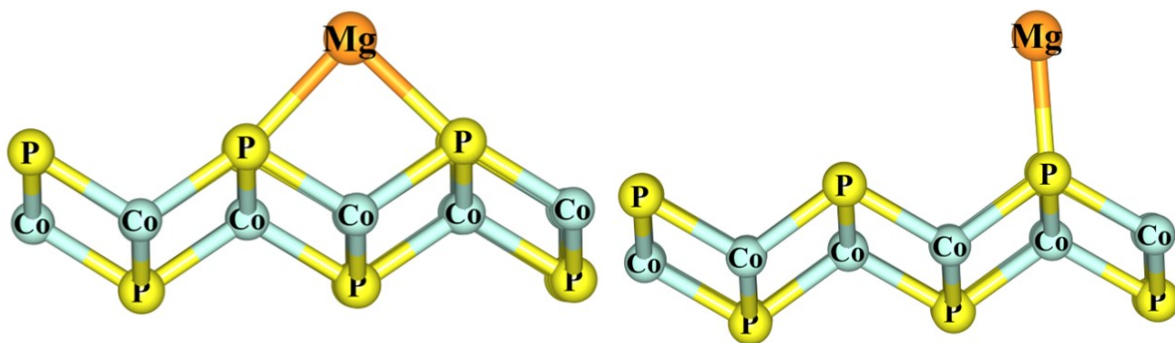


Mg@CoP site 5



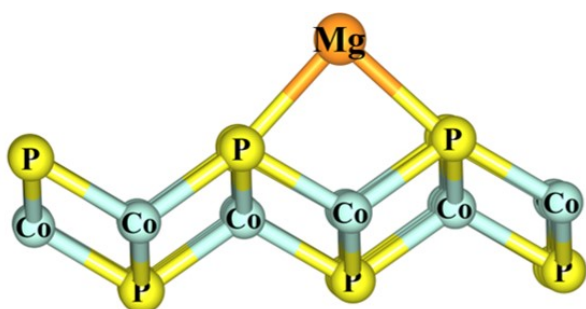
Mg@CoP site 6

Figure S4. The optimized structure of single Mg atom adsorption on CoP anti-MXene at different sites (diglyme condition).

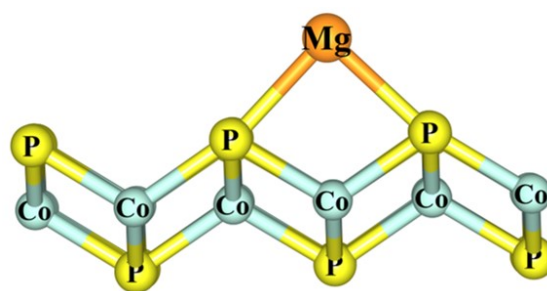


Mg@CoP site 1

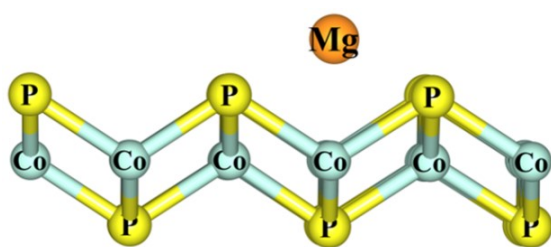
Mg@CoP site 2



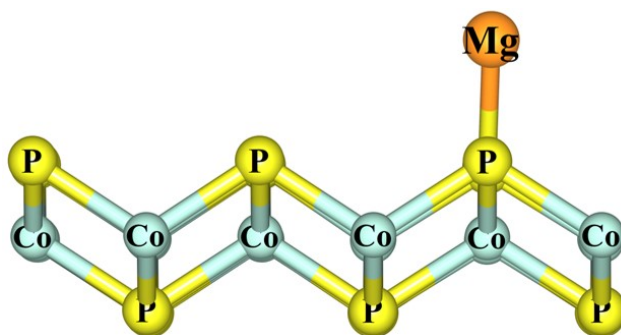
Mg@CoP site 3



Mg@CoP site 4



Mg@CoP site 5



Mg@CoP site 6

Figure S5. The optimized structure of single Mg atom adsorption on CoB anti-MXene at different sites (triglyme condition).

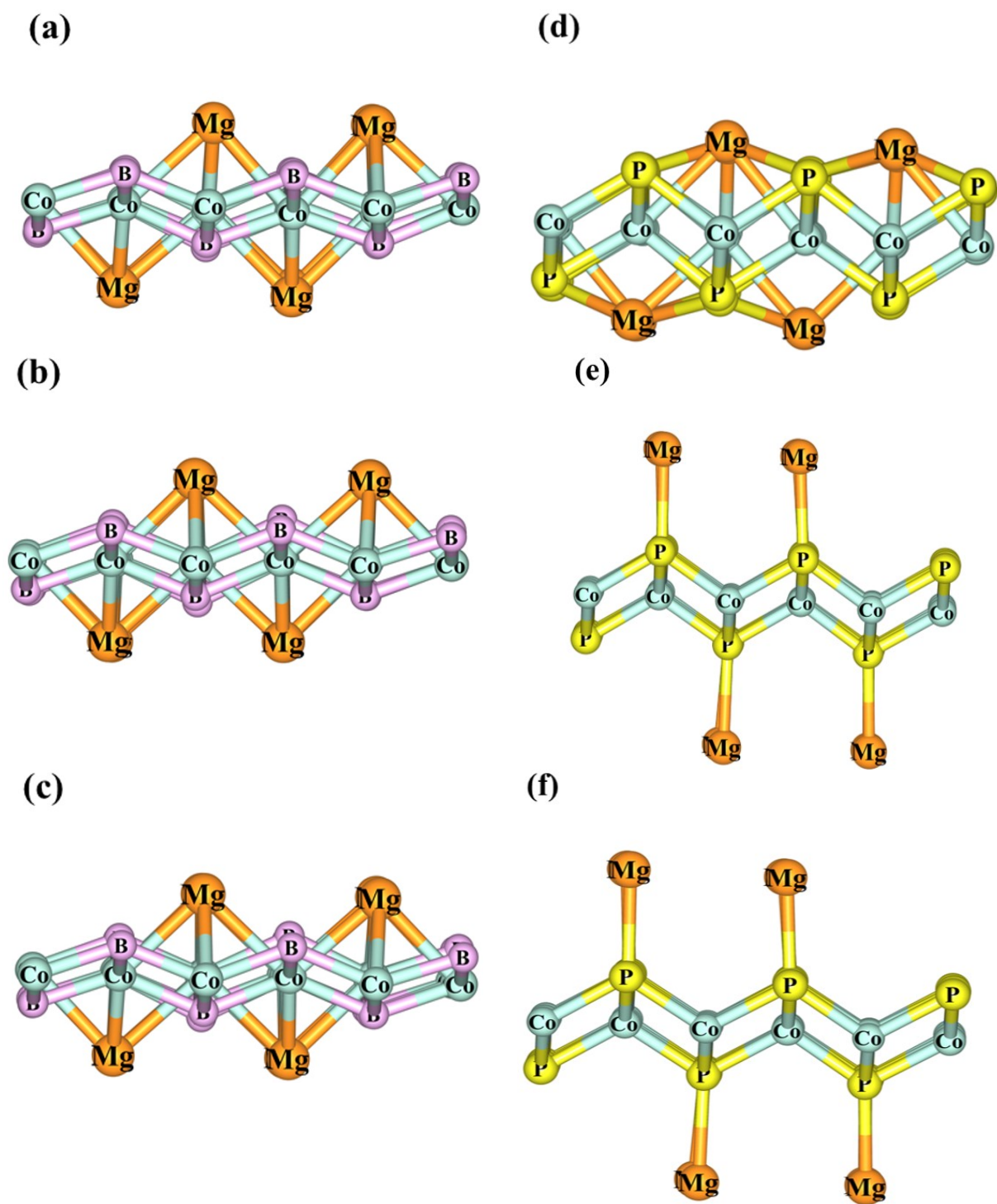


Figure S6. (a-f) depict the optimized structures of $\text{Mg}_8\text{Co}_{18}\text{B}_{18}$ and $\text{Mg}_8\text{Co}_{18}\text{P}_{18}$ systems, respectively for vacuum, diglyme, and triglyme effects.