

Abstract Submitted
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Promoting alkali and alkaline-earth metals on MgO for enhancing CO₂ capture by first-principles calculations HYOSEOK KIM, WON BO LEE, KIWOONG KIM, Sogang Univ — The CO₂ capture properties of Alkali(Li-, Na-, K, Rb-, and Cs-) and Alkaline-Earth metal(Be-, Ca-, Sr-, and Ba-) promoted MgO sorbents are investigated by first principles density functional theory on the basis of PW91/GGA augmented with DFT+D2. Calculated Adsorption energy on the metal-promoted MgO sorbents is higher than Pure MgO sorbents, except for the Na-promoter. These results indicate that the CO₂ capture capacity is improved by metal promotion. Li, Ca, and Sr were identified as adequate promoters among 9 metals, considering bind stability and regenerability

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