

### Promoting Alkali and Alkali -Earth Metals on MgO for Enhancing CO<sub>2</sub> Capture by First -Principles Calculation

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Magnesium oxide (MgO) is a promising sorbent because of its moderate sorption-desorption temperature and low heat of sorption. However, its low sorption capacity and thermal instability need to be improved. Various metal-promoted MgO sorbents have been experimentally developed to enhance the CO<sub>2</sub> sorption capacities. Nevertheless, rigorous computational studies to screen an optimal metal promoter have been limited to date. We conducted first-principles calculations to select metal promoters of MgO sorbents. Five alkali (Li-, Na-, K-, Rb-, Cs-) and 4 alkaline earth metals (Be-, Ca-, Sr-, Ba-) were chosen as a set of promoters. Compared with the CO<sub>2</sub> adsorption energy on pure MgO, the adsorption energy on the metal-promoted MgO sorbents is higher, except that for the Na-promoter, which indicates that metal promoting on MgO is an efficient approach to enhance the sorption capacities. Based on the stabilized binding of promoters on the MgO surface and the regenerability of sorbents, Li, Ca, and Sr were identified as adequate promoters among the 9 metals. The adsorption energies of CO<sub>2</sub> on metal-promoted MgO sorbents for Li, Ca, and Sr atoms are -1.13, -1.68, and -1.48 eV, respectively.