First-principles investigation of CO_2 adsorption on M_1 (M_2)-doped (promoted)-MgO-CaO surface (M_1 = Sr and Ba, M_2 =Li, Na, K, and Rb)

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Global warming has been the one of the most serious environmental problems over the past few decades. Many researchers have made effort to remove CO_2 which is one of the key factors for global heating. Alkaline earth metal oxides have been considered as one of good CO_2 capture materials. For example, MgO is one of the good candidates for CO_2 capture, because of its low operating temperature and regeneration energy [1]. However, CO_2 capacity of MgO is lower than the capacity of CaO [2]. It was reported that the addition of MgO to CaO enhances the structural stability of adsorbents and adsorption capacity of CO_2 [3]. In this study, the CO_2 adsorption on (100) surface of MgO-CaO was investigated by density functional theory (DFT) calculations. Furthermore, dopants (M_1 = Sr and Ba) and promoters (M_2 = Li, Na, K, and Rb) were introduced to the surface to improve the adsorption. Our work will provide the way for designing high-performance metal oxide-based CO_2 adsorbent materials.

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