# First-principles exploration of $M_2O$ (M = Li, Na, and K) for $CO_2$ adsorption

김영섭, 강성구†
울산대학교
(sgkang@ulsan.ac.kr†)

Carbon dioxide ($CO_2$) emitted from fossil fuels is the major gas causing global warming and climate change. There are many different approaches to solve these problems *via* adsorption, absorption, or separation using membranes. In this study, we especially chose three alkali metal oxides, $Li_2O$, $Na_2O$, and $K_2O$ for $CO_2$ adsorption. Using first-principles density functional theory (DFT) calculations, we firstly obtained the adsorption energies of $CO_2$ on dopant-free $Li_2O$, $Na_2O$, and $K_2O$ (111) surface. Then, two different strategies to improve the $CO_2$ adsorption were used. Firstly, we doped other alkali metals on these surfaces to understand the effect of dopants on $CO_2$ adsorption. Secondly, we applied strains (-3 ~ + 3%) to the doped system which has the highest adsorption energy of $CO_2$. To understand the charge transfer between the adsorbent and these systems, Bader charge analysis was carried out. These studies will be helpful to develop an effective adsorbent for $CO_2$ capture.