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Doping Li and K into Na_2ZrO_3 Sorbent to Improve Its CO_2 Capture Capability YUHUA DUAN, DOE-National Energy Technology Laboratory — Carbon dioxide is one of the major combustion products which once released into the air can contribute to global climate change. Solid sorbents have been reported in several previous studies to be promising candidates for CO_2 sorbent applications due to their high CO_2 absorption capacities at moderate working temperatures. However, at a given CO_2 pressure, the turnover temperature (T_t) of an individual solid capture CO_2 reaction is fixed and may be outside the operating temperature range (ΔT_o) for a particularly capture technology. In order to shift such T_t for a solid into the range of ΔT_o, its corresponding thermodynamic property must be changed by changing its structure by reacting (mixing) with other materials or doping with other elements. As an example, by combining thermodynamic database searching with *ab initio* thermodynamics calculations, in this work, we explored the Li- and K-doping effects on the T_t shifts of Na_2ZrO_3 at different doping levels. The obtained results showed that compared to pure Na_2ZrO_3, the Li- and K-doped mixtures $Na_{2-\alpha}M_\alpha ZrO_3$ (M=Li, K) have lower T_t and higher CO_2 capture capacities.

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