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Identifying Solid Sorbents for CO_2 Capture Technology by *ab initio* Thermodynamic Approach YUHUA DUAN, Natl Energy Technology Lab — Since the current technologies for capturing CO_2 are still too energy intensive, to develop new materials that can capture CO_2 reversibly with acceptable energy costs are needed. By combining thermodynamic database mining with first principles density functional theory and phonon lattice dynamics calculations, a theoretical screening methodology to identify the most promising CO_2 sorbent candidates from the vast array of possible solid materials have been proposed and validated. The calculated thermodynamic properties of different classes of solid materials versus temperature and pressure changes were further used to evaluate the equilibrium properties for the CO_2 adsorption/desorption cycles. According to the requirements imposed by the pre- and post- combustion technologies and based on our calculated thermodynamic properties for the CO_2 capture reactions by the solids of interest, we were able to identify only those solid materials for which lower capture energy costs are expected at the desired pressure and temperature conditions. At a given CO_2 pressure, the turnover temperature (T_t) of an individual solid capture CO_2 reaction is fixed. Such T_t may be outside the operating temperature range (ΔT_o) for a particularly capture technology. In order to adjust T_t to fit the practical ΔT_o, in this study, we demonstrate that by mixing different types of solids it's possible to shift T_t to the a range of practical operating temperature conditions.

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