

Abstract Submitted
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Computational designing and screening of solid materials for CO₂ capture YUHUA DUAN, US DOE-Natl Energy Technology Lab — In this presentation, we will update our progress on computational designing and screening of solid materials for CO₂ capture. 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 CO₂ sorbent candidates from the vast array of possible solid materials have been proposed and validated at NETL. The advantage of this method is that it identifies the thermodynamic properties of the CO₂ capture reaction as a function of temperature and pressure without any experimental input beyond crystallographic structural information of the solid phases involved. 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 CO₂ adsorption/desorption cycles. According to the requirements imposed by the pre- and post- combustion technologies and based on our calculated thermodynamic properties for the CO₂ 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 working conditions. In addition, we present a simulation scheme to increase and decrease the turnover temperature (T_t) of solid capturing CO₂ reaction by mixing other solids. Our results also show that some solid sorbents can serve as bi-functional materials: CO₂ sorbent and CO oxidation catalyst. Such dual functionality could be used for removing both CO and CO₂ after water-gas-shift to obtain pure H₂.

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