

Abstract Submitted
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***Ab initio* Thermodynamic Approach to Screen Good Solid Sorbents for CO₂ Capture** YUHUA DUAN, National Energy Technology Lab — CO₂ is the major product from coal combustion and released into the air to cause global climate warming. Current technologies for capturing CO₂ including solvent-based (amines) and CaO-based materials are still too energy intensive. Solid materials have been proposed for capturing CO₂ through a reversible chemical transformation at low cost. By combining DFT with phonon lattice dynamics, the thermodynamic properties of solid materials are obtained and used for computing the thermodynamic reaction equilibrium properties of CO₂ absorption/desorption cycle based on chemical potential and heat of reaction analysis cycle. Based on our calculated thermodynamic properties of reactions for each solid capturing CO₂ varying with T and P, only those solids, which result lower energy cost in the capture and regeneration process and could work at desired conditions, will be selected as promised candidates of CO₂ sorbents and further be sent for experimental validations. Here, we first report our screening results on alkali and alkaline earth metal oxides, hydroxides and carbonates/bicarbonates and compare with available thermodynamic data, then, report the predicted good candidates of CO₂ sorbents from vast of mixing and substituted/doped solids which thermodynamic data are usually not available.

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