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***ab initio* Thermodynamic Approach to Identify Good Solid Sorbents for CO_2 Capture Applications** YUHUA DUAN, National Energy Technology Lab. — By combining thermodynamic database searching with first principles density functional theory and phonon lattice dynamics calculations, a theoretical screening methodology to identify most promising candidates for CO_2 sorbents has been proposed (Duan & Sorescu, PRB(2009), JCP(2010)). For given solids, first we can search their thermodynamic properties from thermodynamic databases and literatures. If their thermodynamic properties are unknown, we perform *ab initio* thermodynamic approach to calculate them out. These properties are used for computing the thermodynamic reaction equilibrium properties of CO_2 absorption/desorption cycle based on the chemical potential and heat of reaction analysis. According to the pre- and post- combustion technologies and conditions in powerplants, based on our calculated thermodynamic properties of reactions for each solid capturing CO_2 varying with temperatures and pressures, only those solid materials, which result lower energy cost in the capture and regeneration process and could work at desired conditions of CO_2 pressure and temperature, will be selected as promised candidates of CO_2 sorbents and further be considered for experimental validations.

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