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 ($\Delta T_o$) for a particularly capture technology. In order to adjust $T_t$ to fit the practical $\Delta T_o$, 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.

Yuhua Duan
Natl Energy Technology Lab

Date submitted: 16 Oct 2013

Electronic form version 1.4