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Large-Scale Computational Screening of Novel Compounds for Carbon Capture

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Carbon capture and storage (CCS) applications offer a plausible solution to the urgent need for a carbon neutral energy source from stationary sources, including power plants and industrial processes. The most mature technology for post-combustion capture currently uses a liquid sorbent, amine scrubbing. However, with the existing technology, a large amount of heat is required for the regeneration of the liquid sorbent, which introduces a substantial energy penalty. Operation at higher temperatures could reduce this energy penalty by allowing the integration of waste heat back into the power cycle. New solid absorbents for use at intermediate to high temperatures, such as CaO, have shown promise in pilot plant studies, but are still far from ideal due to their poor capacity retention upon successive cycling. This presentation will describe our studies aimed at rationally selecting and designing materials for carbon capture and storage applications. We use ab initio calculations of oxide materials from the Materials Project database1 in an effort to screen for novel materials with optimal thermodynamic and kinetic properties for CO2 looping applications. From the determination of a material's optimised structure and ground state energy we have then constructed a screening routine for materials within the database based on simulating their carbonation equilibria and phase stability under differing atmospheric concentrations of CO2. A number of promising materials were identified from the screening, and we are currently investigating their properties experimentally, by using a combination of methods (including thermogravimetric analysis, in situ x-ray diffraction and microscopy). In this way we are able to assess the validity of the screening methodology, and use the insights afforded by experimental studies to iteratively improve the entire process.

[1] *A. Jain, S.P. Ong, G. Hautier, et al, Applied Physics Letters Materials, 2013, 1(1), 011002.*

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