Carbon-ion Conducting Thin Film Membranes Towards Efficient CO_2 Separation
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This one-year seed project aims to design and develop new materials that exclusively transport carbon-ions as a prelude to selective membranes for electrochemical separation and capture of CO_2 from point sources such as coal power plants. Currently, there are no solids known for carbon-ion transport.

None of the commercially available technologies that are currently under consideration for large scale CO_2 separation can offer absolute selectivity or specificity. Most rely on the principles of either differential solubility of CO_2 with respect to other gaseous components, as is the case for polymer membranes and liquid absorption, or differential adsorption of CO_2 in the case of pressure or vacuum swing separation techniques. In other words, these are essentially enrichment or concentration techniques, not selective separation, that require many process cycles to obtain a pure CO_2 steam appropriate for sequestration. Hence, successful demonstration of carbon-ion transport at practically meaningful rates and temperatures in a dense solid will represent a groundbreaking accomplishment.

The materials focus of this project is on doped carbides and involves a two prong strategy that includes both an experimental approach to synthesize appropriate carbide thin films and a computational approach to help guide experimentation and materials selection. In search for a proper methodology to synthesize these materials, we are currently building a specialized reactor for thin film fabrication, doping and testing.

Using the Vienna *Ab Initio* Simulation program (VASP) code and density functional theory (DFT), we calculated the band structure and estimated the band gaps of some of the candidate carbides and compared the efficacy of this approximation by running the program for some materials whose electronic properties are well established. The results pointed to several candidate materials whose band gaps may be suitable for consideration as the host material for doping. It was also possible to propose the chemical identity of the migrating species. More importantly, DFT calculations indicated that the activation barrier for ion migration in some materials may be vanishingly small, suggesting rapid ion transport (i.e., high flux) in such materials. This would be attractive for practical purposes. Work is underway to expand on these preliminary but encouraging results, and determine ion transport rates at practical temperatures.

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