Materials for Alternative Energies: Materials Discovery and Crystal Structure Prediction

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Many of the key technological problems associated with alternative energies may be traced back to the lack of suitable materials. The materials discovery process may be greatly aided by the use of computational methods, particular those atomistic methods based on density functional theory. In this talk, we present an overview of recent work on energy-related materials from density-functional based approaches. We have developed computational tools which enable accurate prediction of crystal structures for new materials (using both Monte Carlo and Genetic Algorithm based approaches), as well as favored lithiation pathways for novel Li battery electrodes. We highlight applications in the area of Li battery materials and hydrogen storage and, time permitting, also briefly discuss our recent research in nanostructured thermoelectric materials, and materials for solar thermochemical water splitting.

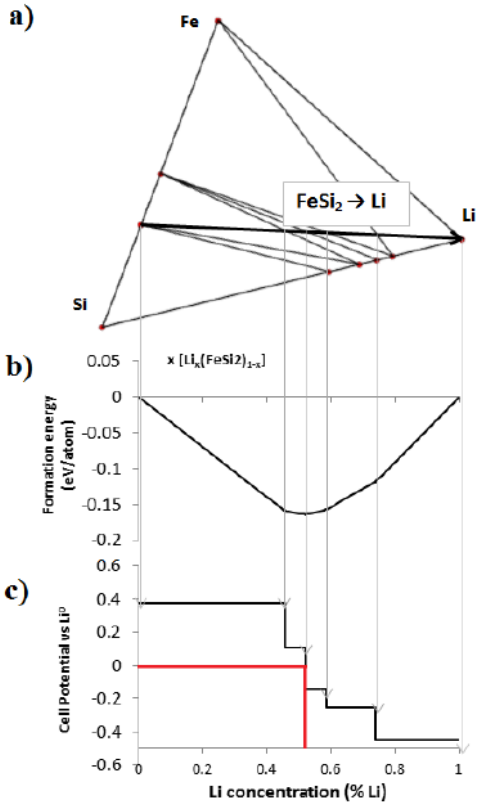

Fig. 1. Step-by-step calculation of the potential-capacity curve of FeSi2 from the first-principles phase diagram. On the ternary phase diagram (a), a lithiation reaction corresponds to the bold line drawn from an initial composition, FeSi2 in this example, straight toward the Li vertex. Along this reaction path, any intersecting tie-line will correspond to a change in the lithiation reaction, and a kink in the convex hull (b). The potential as a function of composition is simply the slope of each segment of the convex hull; therefore the potential-capacity curve (c) will have a step at each kink in the convex hull. The final capacity of the reaction is given by the composition at which the chemical potential of lithium falls below 0, marked by

the red line.

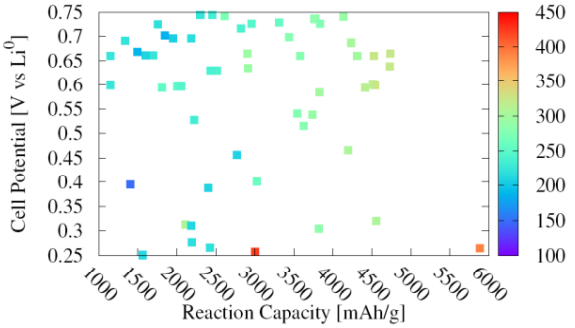

Fig. 2.. High-throughput computational screening of lithiation reactions: Average cell potential, volumetric lithium capacity and volume expansion for every lithiation sequence for transition metal silicides, stannides and phosphides.