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Computational Investigation of Chevrel Phase Cathodes for Ca^{2+} Ion Batteries MANUEL SMEU, Binghamton University - SUNY — While batteries employing Li ions are best suited for applications were portability is important, less expensive alternatives may be employed when size and weight are less critical. Batteries utilizing Ca ions have received very little attention to date due to difficulties in identifying adequate anode materials and electrolytes, although advancements have been made on both fronts. If these challenges can be overcome, Ca can offer an abundant and affordable alternative to Li for grid storage and in other applications where portability is not a priority. For such technologies, appropriate cathodes need to be identified that will allow for reversible intercalation of Ca^{2+} ions and that can provide a desirable voltage. To this end, we investigate the Chevrel phase (CP) compounds Mo_6X_8 (X = S, Se, Te), which can intercalate Mg^{2+} and Ca^{2+}, among many other ions. We use density functional theory (DFT) to calculate the voltage profiles of various guest intercalation ions (Mg, Ca, Sr, Ba) in the CP material. The electronic properties of this material will be discussed, along with the capacity and the energetics associated with ions diffusing through the CP structure. This work also offers insights into how the cathode properties may be fine-tuned by carefully selecting its constituents.

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