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First-Principles evaluation of the Chevrel phase intercalated with Be, Mg, Ca, Sr, and Ba TAYLOR JURAN, MANUEL SMEU, Binghamton Univ — Li ion batteries are extremely useful when an item requires portability and compactness, such as laptops and cell phones; due to the lightweight/compact nature of Li ion batteries. The lightweight and compact nature of Li ion batteries comes at a high cost. It is sensible to consider Li ion battery alternatives, which are more cost effective and useable when portability is not a priority. An option for a less expensive battery source is the Ca ion battery. The Ca ion battery is interesting as many researchers overlook the potential battery source due to the perplexity of finding suitable anode materials and electrolytes. In order for this technology to work, cathodes that allow for the reversible intercalation of Ca^{2+} ions and also provide a preferred voltage must be identified. We investigate the Chevrel phase compounds of Mo_6X_8 (X = S, Se, Te) which can intercalate various ions. The concentration of the ion intercalated with the Chevrel cathode is studied. We consider doped versions of the Chevrel phase, using various dopants to substitute Mo. We use density functional theory to calculate the voltage of several intercalation ions with the Chevrel material. The resulting electronic properties of the aforementioned materials will be investigated.

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