First-principles search for potential high temperature superconductors in the Mg-B-A (A=alkaline metal) system with high boron content\textsuperscript{1} ROMAN CHEPULSKYY, Duke University, IGOR MAZIN, Naval Research Laboratory, STEFANO CURTAROLO, Duke University — Possible superconductivity at 50K was recently reported \cite{1} in the Mg-B-A (A=Cs, Rb, Ba) system. Although attempts to reproduce this finding have been unsuccessful so far \cite{2}, if a stable or metastable phase could be found by a first principle search similar to that in Ref. 3, this would have lent credibility to the experimental finding \cite{1} and outline possible further directions. The results of Ref. 1 suggest that (a) the superconducting phase is not similar to MgB\textsubscript{2} (B site has cubic or similarly high symmetry) and (b) boron content is higher than in MgB\textsubscript{2}. We report first-principles study of the thermodynamics of alkali and alkaline earth doping in the boron-rich part of the Mg-B phase diagram (MgB\textsubscript{n} with \(n \geq 2\)), searching for a phase that could explain the results of Ref. \cite{1}. \cite{1} A.V. Palnichenko \textit{et al.}, JETP Letters \textbf{86}, 272 (2007). \cite{2} R K Singh \textit{et al} http://arxiv.org/abs/0709.4001v1. \cite{3} S. Curtarolo \textit{et al}, Calphad \textbf{29}, 163 (2005).

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