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First-principles search for potential high temperature superconductors in the Mg-B-A (A=alkaline metal) system with high boron content[1] ROMAN CHEPULSKYY, Duke University, IGOR MAZIN, Naval Research Laboratory, STEFANO CURTAROLO, Duke University — Possible superconductivity at 50K was recently reported [1] in the Mg-B-A (A=Cs, Rb, Ba) system. Although attempts to reproduce this finding have been unsuccessful so far [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 [1] and outline possible further directions. The results of Ref. 1 suggest that (a) the superconducting phase is not similar to MgB_2 (B site has cubic or similarly high symmetry) and (b) boron content is higher than in MgB_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_n with $n > 2$), searching for a phase that could explain the results of Ref. [1]. [1] A.V. Palnichenko *et al.*, JETP Letters **86**, 272 (2007). [2] R K Singh *et al* http://arxiv.org/abs/0709.4001v1. [3] S. Curtarolo *et al*, Calphad **29**, 163 (2005).

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Roman Chepulskyy
Duke University

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