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Prediction of new crystal structure phases in metal borides

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Identification of novel crystal structures is an important step for predicting new stable compounds in alloys, since most theoretical search algorithms are restricted to a given prototype library or a lattice type. Performing *ab initio* data mining [1] of intermetallic compounds we have discovered that even in such a well-studied class of systems as metal borides there are previously unknown phases comparable in energy to the existing ones [2]. We demonstrate that even though the new structures are relatively simple, their identification is not straightforward. We systematically investigate the stability and electronic properties of the new metal boride phases. Our calculations show that some phases exhibit electronic features similar to those in the famous MgB_2 and could be good superconductors. The new phases are likely to have random stacking faults, so they might not be detected with standard x-ray methods. Our results could thus be used as an important guide in the search for new superconducting metal borides. [1] S. Curtarolo *et al.*, Phys. Rev. Lett. **91**, 135503 (2003). [2] A.N. Kolmogorov *et al.*, submitted (2005).