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New Stable Phases in the Re-B System: A First-principles Study
XIN ZHAO, MANH CUONG NGUYEN, CAI-ZHUANG WANG, KAI-MING HO, Iowa State University, IOWA STATE UNIVERSITY TEAM — We studied rhenium borides using genetic algorithm in combination with first-principles calculations and revealed several new stable phases in the Re-B system. The structures obtained from our genetic algorithm search are energetically much superior to those proposed in the literature. Two new phases of Re2B were found to be thermodynamically stable at different pressures, which possibly explains the recent experimental observations (Solid State Sciences 25 85-92 (2013)). ReB is stable against decomposition reactions below 10 GPa and ReB3 is stable above 22 GPa. A C2/m structure was discovered for ReB4 to have lower energy than the R-3m structure reported earlier (J. Alloys Compd. 573 20-26 (2013)). Elastic properties from first-principles calculations indicate that the structures we report in this work are mechanically stable and promising targets as new ultra-hard materials.

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