

Abstract Submitted
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Magnesium phase diagrams: Have you seen us? GUS HART, Brigham Young University, STEFANO CURTAROLO, Duke University — Because of its high strength-to-weight ratio, magnesium is seen as promising material for automotive applications. But magnesium alloys are far less understood than more common alloys such as steel or newer alloys such as aluminum. Even among simple binary magnesium systems, there is a great deal of missing information. There are binary magnesium systems for which no phase diagrams appear in the latest databases (the Pauling File, for example). Using a high-throughput approach, we have undertaken a broad search for ground states in 40 magnesium binary systems using more than 8000 fully-relaxed first-principles calculations. We find new, non-obvious ordering systems and many systems where there are unsuspected ground states. We discuss the results and their potential impact on magnesium alloys.

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