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Binary Magnesium Alloys: Searching for Novel Compounds by Computational Thermodynamics RICHARD TAYLOR, STEFANO CURTAROLO, Duke University, GUS HART, Brigham Young University — Magnesium alloys are among the lightest structural materials and are of considerable technical interest. We use the high-throughput framework AFLOW to make T = 0 K ground state predictions by scanning a large set of known candidate structures for thermodynamic minima. The study presented here encompasses 34 Mg-X systems of interest (X=Al, Au, Ca, Cd, Cu, Fe, Ge, Hg, Ir, K, La, Pb, Pd, Pt, Mo, Na, Nb, Os, Rb, Re, Rh, Ru, Sc, Si, Sn, Sr, Ta, Tc, Ti, V, W, Y, Zn, Zr). Avenues for further investigation revealed by this study include stable phases found in addition to experimental phases and compound forming systems thought to be either immiscible or non-compound forming. The existence of potentially novel ordered phases presents new opportunities for materials design.

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