

Abstract Submitted
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Where are Nature's missing structures? GUS HART — It has long been claimed that predicting crystal structures of compounds using “first-principles” (direct solution of the Schoedinger equation using computers) will fundamentally change the way new materials discoveries are made. However, the ability to reliably predict new materials has been elusive. This ability is elusive for two reasons: the enormous search space of possible crystal structures and the relatively long times required for calculations of candidate materials. In this talk, I will discuss the problem from a different angle: what intermetallic structures are likely based just on simple combinatoric arguments? Some of these likely candidates are indeed well-known intermetallic structures but many other are conspicuously absent. What are the physical reasons that some of these structures exist in Nature and others don't?

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