

Abstract Submitted
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Theory-driven discovery of an exotic CaB₆ high-pressure crystal structure phase ALEKSEY KOLMOGOROV, Binghamton University, SUNY, SHEENA SHAH, ELENA MARGINE, University of Oxford, ANNETTE KLEPPE, Diamond Light Source, ANDREW JEPHCOAT, University of Oxford — We synthesized and solved an unexpectedly complex crystal structure of CaB₆ under high pressures and temperatures [1]. The only known crystal structure in the large family of metal hexaborides, a simple cubic cP7 type, has been shown to transform into a tetragonal tI56 configuration comprised of unfamiliar 24-atom boron units above 30 GPa and remain metastable under ambient pressure. The interpretation of the convoluted x-ray diffraction pattern was accomplished with an ab initio evolutionary search implemented in MAISE [2] which identified the tI56 structure (28 atoms per primitive unit cell) without any parameter input, i.e. truly “from scratch.” I will describe the performance of different ground state search techniques in such challenging cases.

[1] A.N. Kolmogorov et al., Phys. Rev. Lett. 109, 075501 (2012)

[2] Module for Ab Initio Structure Evolution, <http://maise-guide.org>

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