Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

A possible analog to MgB_2: Discovery of a predicted layered LiB via cold compression[1] ALEKSEY KOLMOGOROV, SAMAD HAJINAZAR, CHRIS ANGYAL, Binghamton University, VLADIMIR KUZNETZOV, University of Oxford, ANDREW JEPHCOAT, Okayama University — Stoichiometric LiB has been previously predicted [1,2] to be a new synthesizable layered material with electronic and vibrational properties desired for MgB_2-type superconductivity. However, previous experiments showed no signs of the proposed compound forming under high pressures. We report on the synthesis of the LiB via cold compression in the diamond anvil cell [3]. Remarkably, the signature powder XRD peak from the new layered compound appeared above 21 GPa and remained visible down to ambient pressure upon sample quenching. Apparent stacking disorder in LiB and a stoichiometry shift in the starting LiB_y (from $y \approx 0.90$ down to $y \approx 0.75$) made material characterization a challenge. *Ab initio* modeling allowed us to establish the pressure-dependent composition of LiB_y and predict related stable structures overlooked in previous studies. [1] A.N. Kolmogorov and S. Curtarolo, Phys. Rev. B 74, 224507 (2006) [2] A.N. Kolmogorov and S. Curtarolo, Phys. Rev. B 73, 180501(R) (2006) [3] A.N. Kolmogorov, S. Hajinazar, C. Angyal, V.L. Kuznetsov, and A.P. Jephcoat, Phys. Rev. B 92, 144110 (2015)

[1]Supported by NSF Grant DMR-1410514

Aleksey Kolmogorov
Binghamton University

Date submitted: 05 Nov 2015 Electronic form version 1.4