Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Search for high-Tc conventional superconductivity at megabar pressures in the lithium-sulfur system LILIA BOERI, CHRISTIAN KOKAIL, Graz Univ of Technology, CHRISTOPH HEIL, 2Department of Materials, University of Oxford, Parks Road, Oxford OX1 P3H, United Kingdom — Motivated by the recent report of superconductivity above 200 K in ultra-dense hydrogen sulfide, we search for high-T_c conventional superconductivity in the phase diagram of the binary Li-S system, using ab initio methods for crystal structure prediction and linear response calculations for the electron-phonon coupling. We find that at pressures higher than 20 GPa, several new compositions, besides the known Li_2S, are stabilized; many exhibit electride-like interstitial charge localization observed in other alkali-metal compounds. Of all predicted phases, only an fcc phase of Li_3S, metastable before 640 GPa, exhibits a sizable T_c, in contrast to what is observed in sulfur and phosphorus hydrides, where several stoichiometries lead to high T_c. We attribute this difference to $2s$-$2p$ hybridization and avoided core overlap, and predict similar behavior for other alkali-metal compounds. [1] C. Kokail, C. Heil and L. Boeri, Phys. Rev. B 94, 060502 (R) (2016)

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Date submitted: 10 Nov 2016 Electronic form version 1.4