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Engineering superconductors with ab initio methods: ternary metal borides ALEKSEY KOLMOGOROV, University of Oxford, MATTEO CALANDRA, STEFANO CURTAROLO — We have performed a targeted search for novel superconducting ternary borides starting from the recently identified class of binary metal sandwich (MS) structures [1]. Our *ab initio* calculations suggest that a theoretically-devised MS lithium monoboride gains in stability when alloyed with electron-rich metals [2,3]. In an effort to pre-select compounds with the strongest electron-phonon coupling we evaluate the softening of the in-plane boron phonon mode in a large class of metal borides. Our results reveal interesting general trends for the frequency of the in-plane boron phonons as a function of the boron-boron bond length and the valence of the metal [4]. Research supported by ONR and NSF. [1] PRB 73, 180501(R) (2006) [2] PRB 74, 224507 (2006). [3] PRB 75, 144506 (2007) [4] A.N. Kolmogorov, M. Calandra, S. Curtarolo, submitted to PRB.

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