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Ab initio study of topological phases of lithium at high pressures STEPHANIE MACK, Department of Physics, UC Berkeley, SINEAD GRIFFIN, Department of Physics, UC Berkeley; Molecular Foundry, LBNL, JEFFREY NEATON, Department of Physics, UC Berkeley; Molecular Foundry, LBNL; Kavli Energy NanoScience Institute — Solid lithium under high but experimentally achievable pressures is known to exhibit a rich landscape of phases beyond what is expected for a "simple" metal. Notably, lithium adopts increasingly lower-symmetry phases with increasing density [1] rather than retaining close-packed structures, possibly even culminating in a paired phase. As the overlap between neighboring lithium core states increases, Pauli exclusion and orthogonality force valence electrons into the interstitial regions, driving phase transitions to lower symmetry structures [2,3] and the onset of semi-metallic behavior [3,4]. Using first-principles calculations, we show that the electronic structure of theoretically predicted phases exhibit massless Dirac fermions at the Fermi energy. We explore the possibility of nontrivial topological properties in other lithium phases and extend our study to high-pressure phases of other alkali metals. [1] Guillaume et al., Nat. Phys. 7, 211 (2011) [2] Neaton and Ashcroft, Nature 400, 141 (1999) [3] Marqués et al., PRL 106, 095502 (2011) [4] Matsuoka et al., PRB 89, 144103 (2014)

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