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Nature of Pressure-induced Insulating States in Simple Metals
IVAN NAUMOV, RUSSELL HEMLEY, Carnegie Institution of Washington — As experimentally established, all the alkali metals and heavy alkaline earth metals (Ca, Sr and Ba) become progressively less conductive on compression, at least up to some critical limit over a broad pressure range. Of these metals, Li and Na clearly undergo pressure-induced metal-insulator transitions, which may also be called reverse Mott transitions. Here, using group theory arguments and first-principles calculations, we show that such transitions can be understood in terms of band representations introduced by Zak. The valence bands in the insulating states are described by simple and composite band representations constructed from localized Wannier functions centered on points unoccupied by atoms [1]. The character of the Wannier functions is closely related to the degree of s-p(-d) hybridization and reflects multi-center chemical bonding in these insulating states. The conditions under which an insulating state is allowed for structures having an integer number of atoms per primitive unit cell as well as re-entrant (i.e., metal-insulator-metal) transition sequences are detailed, resulting in predictions of semimetallic phases with flat surface states. The general principles developed are tested and applied to the alkali and alkaline earth metals, including elements where high-pressure insulating phases have been identified or reported (e.g., Li, Na, and Ca). This research was supported by EFree, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award DESC0001057. [1] I. I. Naumov and R. J. Hemley, PRL, **114**, 156403 (2015).

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