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The breakdown of a simple-metal paradigm at high pressures[1]
BRUNO ROUSSEAU, NEIL W. ASHCROFT, Cornell University — The light alkalis at one bar and room temperature are considered the paradigms of 'simple-metal' behavior. They adopt cubic structures and their valence bands are free electron-like. Under normal conditions this has been well accounted for by pseudopotential theory. It is a common expectation that the light alkalis might even be more free electron-like at higher densities, as impelled by pressure. Advances in diamond anvil cell methods have yielded new insights in the behavior of the alkalis at megabar pressures, presenting a considerable challenge to the above paradigm. Under pressure, the light alkalis adopt non-simple structures. Initial studies by Neaton and Ashcroft [Letters to Nature, Vol. 400, 141 (1999)] on lithium suggested that with increasing pressure the valence bands first broaden, but then start narrowing substantially. Corresponding to this, the valence charge density is localizing in the interstitial spaces of the lattice and the core bands are acquiring significant width. Our work focuses on showing that this behavior may be fairly general and can be explained at the one electron level as an emerging breakdown of the weak pseudopotential hypothesis.

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