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Strongly correlated valence electrons and core-level chemical bonding of Lithium at terapascal pressures ANGUANG HU, FAN ZHANG, Defence Research and Development Canada at Suffield Research Centre — As the simplest pure metal, lithium exhibits some novel properties on electrical conductivity and crystal structures under high pressure. All-electron density functional theory simulations, recently developed by using the linear combination of localized Slater atomic orbitals, revealed that the bandwidth of its valence bands remains almost unchanged within about 3.5 eV even up to a terapascal pressure range. This indicates that the development from delocalized to strongly correlated electronic systems takes place under compression, resulting in metal-semiconductor and superconductivity transitions together with a sequence of new high-pressure crystal phases, discovered experimentally. In contrast to the valence bands, the core-level bands become broadening up to about 10 eV at terapascal pressures. It means the transformation from chemical non-bonding to bonding for core electrons. Thus, dense lithium under compression can be characterized as core-level chemical bonding and a completely new class of strongly correlated materials with narrow bands filled in s-electron shells only.

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