

Abstract Submitted
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Electride-like phases at extreme compression: towards bridging the gap between theory and experiment¹ STANIMIR BONEV, Lawrence Livermore National Laboratory — The transformation of materials into electride-like structures under the application of extreme pressure has attracted a lot of interest recently. Theoretical studies have predicted the existence of low-coordinated crystal phases, where the conduction electrons are localized in the interstitial atomic regions, for a number of elements at high density. Most of these works have been limited to static lattice calculations. The pressures where such transformations are projected to occur are accessible in shock-wave experiments, but at elevated temperatures. In this talk I will discuss the temperature dependence of electride structures, both solids and liquids, as well as the requirements for their accurate simulation.

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