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Electride-like phases at extreme compression and elevated temperatures¹ STANIMIR BONEV, Lawrence Livermore National Laboratory, JONATHAN DUBOIS, Lawrence Livermore National Laboratory, Livermore, CA 94550 — The transformation of materials into electrider-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 electrider structures, both solids and liquids, as well as the requirements for their accurate simulation.

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