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Temperature-induced changes in hP4-Sodium Electride: An Ab Initio Study[1] REETAM PAUL, SUXING HU, VALENTIN KARASIEV, Laboratory for Laser Energetics, STANIMIR BONEV, Lawrence Livermore National Laboratory — Crystalline alkali metals generally exhibit near free-electron behavior at ambient conditions. For sodium at high pressures, a deviation from such a metallic behavior was found in the hP4 phase. Diamond anvil cell experiments and associated cold curve calculations have concluded that this change is caused by the formation of hP4 electrides with interstitially localized electrons, which renders this phase transparent. However, higher temperature solid-states accessible by ramp-compression have showed results to the contrary. In this work, we investigate the subtleties of the electronic and optical property changes in such a system with increasing temperatures, using density functional theory with the Kubo-Greenwood formulation. The properties looked into include, among others, the electron localization function, frequency-dependent conductivity, density of electronic states, and electronic band structure for a quantitative explanation of the causes for the emergence of reflectivity in hP4-sodium under high pressure–temperature conditions.

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