Abstract Submitted
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Compression-Driven Enhancement of Electronic Correlations in Simple Alkali Metals[1] GILBERTO FABBRIS, Argonne National Lab./Washington University in St. Louis, JINHYUK LIM, Washington University in St. Louis, LARISSA VEIGA, Argonne National Lab./Brazilian Synchrotron Light Lab., DANIEL HASKEL, Argonne National Lab., JAMES SCHILLING, Washington University in St. Louis — Alkali metals are the best realization of the nearly free electron model. This scenario appears to change dramatically as the alkalis are subjected to extreme pressure, leading to unexpected properties such as the departure from metallic behavior in Li and Na, and the occurrence of remarkable low-symmetry crystal structures in all alkalis. Although the mechanism behind these phase transitions is currently under debate, these are believed to be electronically driven. In this study the high-pressure electronic and structural ground state of Rb and Cs was investigated through low temperature XANES and XRD measurements combined with *ab initio* calculations. The results indicate that the pressure-induced localization of the conduction band triggers a Peierls-like mechanism, inducing the low symmetry phases. This localization process is evident by the pressure-driven increase in the number of *d* electrons, which takes place through strong *spd* hybridization. These experimental results indicate that compression turns the heavy alkali metals into strongly correlated electron systems.

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