Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Metallic surface states in elemental high-pressure electrides IVAN NAUMOV, Carnegie Institution of Washington, RUSSELL HEMLEY, The George Washington University and Lawrence Livermore National Laboratory — In their high-pressure insulating electride phases, the alkali metals Li, Na, and K are unique insulating materials that can be considered as both ionic and covalent. Using a Berry phase analysis we show that such dual chemical character leads to two types of metallic surface states depending on surface termination/orientation. As covalent materials with an inverted $s-p$ bulk band gap, these high-pressure electrides tend to form metallic Shockley-type surface states within the gap. On the other hand, as ionic materials, they have polar surfaces that exhibit metallic surface states due to "electronic reconstruction" in which the electrons move from the valence band on one surface to the conduction band at the opposite surface, thereby making both the surfaces metallic. The results provide predictions for future measurements. This research was supported by EFree, an Energy Frontier Research Center funded by the U.S. DOE, Office of Science, Basic Energy Sciences (award DE-SC0001057). The infrastructure and facilities used were supported by the U.S. DOE/NNSA (award DE-NA-0002006, CDAC). Work at LLNL was performed under the auspices of the DOE (contract DE-AC52-07NA27344).

Ivan Naumov
Carnegie Institution of Washington

Date submitted: 10 Nov 2016 Electronic form version 1.4