Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

First-principles calculation of K absorption edge of warm dense aluminum SHEN ZHANG, WEI KANG, PING ZHANG, X. T. HE, Center for Applied Physics and Technology, Peking University — Shifts of K absorption edge of warm dense aluminum with respect to the change of thermodynamic conditions are calculated using first-principles methods[1], which shows good agreement with the experimental measurements[2]. Improvement is achieved with a careful consideration of the effect of core electrons. The shift of K edge is revealed more sensitive to the change of temperature than to that of density in the warm dense region, which suggests K edge shift a good temperature indicator. The flattening point of the K edge shift at higher temperature is attributed to the thermal depletion of the M-band electrons.

[1]S. Zhang, S. Zhao, W. Kang, P. Zhang, and X. T. He, Phys. Rev. B **93**, 115114 (2016)
[2]A. Benuzzi-Mounaix, F. Dorchies, V. Recoules, F. Festa, O. Peyrusse, A. Levy, A. Ravasio, T. Hall, M. Koenig, N. Amadou, E. Brambrink, and S. Mazevet, Phys. Rev. Lett. **107**, 165006 (2011)

Shen Zhang
Center for Applied Physics and Technology, Peking University

Date submitted: 10 Nov 2016 Electronic form version 1.4