CFEL SCIENCE

SEMINAR

22nd April 2020 - 10:00 a.m.

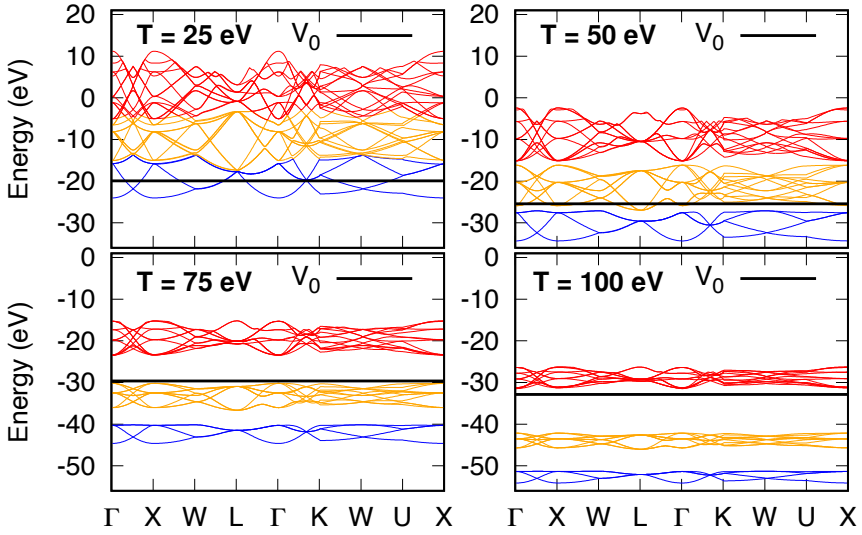
Virtual meeting room in ZOOM (ID: 754 722 433 / PW: 021149)

John Jasper Bekx

Center for Free-Electron Laser Science, DESY, Germany

Electronic-structure calculations for nonisothermal warm dense matter

We present the methodology employed in, and the first results obtained with, the new computational toolkit XCRYSTAL. XCRYSTAL describes the electronic states present in a nonisothermal transient warm-dense-matter (WDM) state created during the first 10–100 fs after the irradiation of a solid sample with an intense femtosecond x-ray pulse. It utilizes a hybrid basis consisting of plane waves and localized core orbitals for high computational efficiency. The core orbitals in the basis are allowed to respond to the presence of plasma electrons through an interwoven inner-shell–outer-shell optimization scheme employed in XCRYSTAL. We compare our result for the *K*-shell threshold energy of solid-density aluminum at WDM conditions with experiment, and obtain values for the orbital-specific ionization potential depression of this system. We will comment on the applicability of the average-atom model in this context, and on the effects of incorporating the full crystal structure as well as the responsive core orbitals. Furthermore, we will present temperature-dependent band structure predictions for this transient nonisothermal WDM system.



Band structure of Al at WDM conditions

Host: Robin Santra – CFEL-DESY Theory Division