Contribution ID: 33

Comparisons of density-functional average-atom models and measures of the mean ionization state

Monday 21 February 2022 17:10 (20 minutes)

Average-atom (AA) models are an important tool in the modelling of warm dense matter, being both a computationally cheap and conceptually straightforward alternative to full DFT MD simulations. AA models are typically based on a common premise - namely, an atom immersed in a plasma environment - but use a range of different assumptions and approximations, which can cause inconsistent predictions for various properties. In this talk, I will compare results across several models, differing for example in their choice of boundary conditions and exchange-correlation functional. I will focus on the mean ionization state (MIS), an important property in WDM. I will compare different methods for computing the MIS, including methods which are historically popular and still widely-used in AA codes, and also consider more novel approaches using the electron localization function and Kubo-Greenwood formalism. If time permits, these results with also be compared with results from full DFT-MD simulations.

Primary author: CALLOW, Timothy (CASUS, HZDR)

Co-authors: KRAISLER, Eli (Hebrew University of Jersulam); Dr CANGI, Attila (Center for Advanced Systems Understanding, HZDR)

Presenter: CALLOW, Timothy (CASUS, HZDR)

Session Classification: Session 2