Metals at high pressure and high temperature: Following the electronic structure using X-Ray Absorption Spectroscopy

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The study of the so-called Warm Dense Matter (WDM) is a challenging field that is at the crossroads of condensed matter and plasma physics. Here the density goes from one percent of the solid density up to 10 times its value; the temperature varies from 0.1 to 100 eV. In this regime, matter is mostly degenerate, strongly coupled and non-ideal. Great uncertainties remain regarding the physics of these states of matter. X-ray Absorption Near Edge spectra (XANES) brings invaluable information on the evolution of the electronic structure as the system is subject to a significant increase in both pressure and temperature to reach this WDM regime.

From the theoretical side, the use of ab initio electronic structure approach based on Density Functional Theory combined with molecular dynamics simulations and linear response theory has been rather successful at providing a satisfying description of equation of states and transport properties of this complex regime. X-ray absorption for warm dense matter is a new field of applications for this approach. Using this method, the density and temperature variations of the XANES spectra has been computed for warm dense aluminium, iron, molybdenum and copper. The dramatic change in the structural properties of the system results in significant variations of the overall XANES spectrum as well as measurable energy shifts due to the change in density and/or temperature. The strong interaction with experiment all along these projects enable us to show how XANES spectra can be used to diagnose solid-solid and solid-liquid phase transition and to follow the evolution of the electronic structure during phase transition.

Der Gast wird betreut von Frau Prof. B. Rethfeld
Gäste sind herzlich willkommen
Kaffeeausschank ab 17:00 Uhr

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