



INTERDISCIPLINARY CENTRE FOR  
ADVANCED MATERIALS SIMULATION

## ICAMS Seminar

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Monday, May 7, 4:30 p.m. ICAMS Seminar room UHW 11/1102

High pressure stability of transition metals: recent developments from first principles  
thermodynamics

The thermodynamic stability of solids and liquids under high pressure and temperature conditions is a topic of intense research activity. Particularly interesting is the on-going controversy on the crystal structure and melting curve of various transition metals including Mo, Ta and to a lesser extent Fe. On the experimental side, the most striking differences appear when diamond anvil cell experiments are compared to shock wave experiments. On the theoretical side differences are apparently related to different theoretical methods and their applications. In this talk I will present a recent analysis of some of these methods, including the free energy method, the coexistence of phases and the recently proposed "Z" method. I will show that when applied in a consistent way they all predict the same melting properties and crystal structure stability, and I will discuss the balance of advantages and disadvantages of each method. Results will be presented for Fe, Ta and Mo. In particular, our calculations for the case of Mo show that it probably melts from the body centred cubic phase and has a high melting curve, compatible with shock wave experiments.

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