CELOÚSTAVNÍ SEMINÁŘ
Ústavu fyziky materiálů AV ČR

dne **30.1.2012** (pondělí) ve **14:00 h**
v přednáškovém sále (4. patro)
Ústavu fyziky materiálů AV ČR, Žižkova 22, Brno

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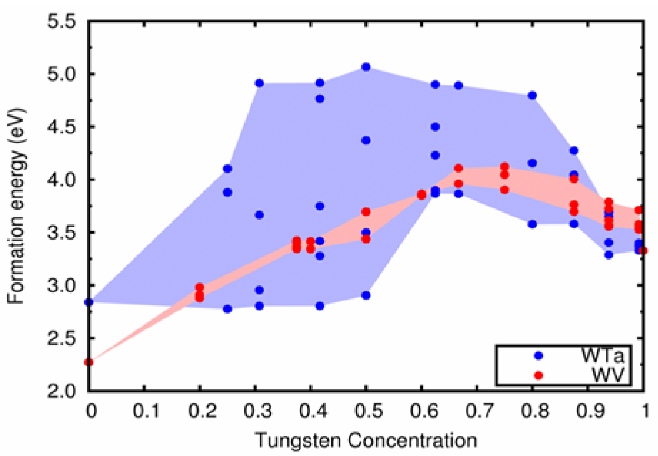
Advances in Multi-scale Modeling of Structural Stability and Radiation Defects in Materials for Nuclear Fusion Power Plants

Fusion – along with solar power and fission reactors – is the only feasible way to fill the gap between the energy available from conventional fossil fuels and the ever-rising total global energy demand. Developing predictive schemes to understand structure and mobility of defects under neutron irradiation in these materials (that are mostly based on bcc transition metals) is essential for modeling micro-structural evolution of fusion materials. Our recent systematic and multi-scale studies based on density functional theory (DFT) calculations of self-interstitial atom (SIA) defects, spanning the entire group of bcc metals, reveal that the SIAs adopt a linear <111> crowdion configuration in all non-magnetic bcc transition metals whereas in ferromagnetic iron the most stable SIA configuration has the <110> orientation. The predicted SIA formation energy in bcc-W has been recently confirmed experimentally. Fe-Cr alloys-based ferritic/materrensitic steels represents a great challenge in computational materials science because the magnetic interactions involving both constituent elements of the alloy give rise to a fairly complex picture of phase transitions, including the fundamental mechanisms of α' (bcc-Cr) precipitation and kinetic phase transformation at finite temperature. Here, we present two complementary approaches based on ab-initio density functional theory (DFT) calculations in order to predict the magnetic behavior in this frustrated system. Applying these models to studying irradiated defect properties, it is shown that this model is able to predict very complex magnetic configurations not only for self-interstitial atom (SIA) dumbbells but also for the 1/2[111] screw dislocations. Finally I will present some new results related to our current first-principles investigation of point defects in W alloys for fusion power plant application (see Figure below).



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