Ph.D thesis position at CEA Saclay, France

Carbides in ferritic steels: from electronic structure to thermodynamics

Carbide formation is well known to drastically change the mechanical properties of steels. This phenomenon has a fundamental impact when steels are used as structural materials for numerous technological applications. In particular, the presence of carbides in current generation of nuclear reactors (Gen II and Gen III), especially in heavy forging components such as vessel or steam generators, may induce serious safety concerns.

This thesis is part of a multi-scale and coupled experimental-theoretical project, which aims at investigating the interplay between chemical composition, microstructure and mechanical properties of model steels containing solutes, such as Mo, Mn and Cr, that favor the formation of carbides.

The objective of this thesis is to interpret the experimentally observed sequence of emerging carbides as a function of temperature and composition of the model steels, and to provide information not directly accessible by experiments, using a combination of electronic-structure and thermodynamic (CALPHAD) approaches.

To reach the end, first-principles electronic-structure calculations (based on density functional theory: DFT) will be carried. They provide the electronic- and atomic-scale driving forces at the origin of the relative stability of various carbide phases, either observed experimentally or predicted by CALPHAD thermodynamic models. They also allow predictions of carbide structures and stabilities as functions of the solute concentrations, as well as the nucleation mechanisms of the carbides (critical size, coherence-incoherence transition etc.). Finally, the obtained DFT data are useful to either validate or improve the CALPHAD prediction of carbide properties (especially for moderate and low temperatures), which often relies on extrapolations of high temperature data from experiments.

Highly motivated candidates holding a Master degree in the field of Solid State Physics or Materials Science are encouraged to apply. Experience in atomistic simulation and expertise in coding are highly appreciated.

Interested candidates are invited to contact Dr. Chu-Chun FU (chuchun.fu@cea.fr) , providing the CV and a letter of motivation.