2-year postdoctoral position

Modeling of Ti-Zr-O thermodynamics from ab initio calculations

A postdoctoral position is available in the laboratory of physical metallurgy in CEA Saclay (France) for two years starting this Fall 2020.

Among the various significant questions affecting titanium metallurgy, the effect of oxygen on the mechanical properties of titanium alloys remains one of the most critical issues. A small addition of oxygen is known to induce a strong hardening resulting in a large increase of strength but also a drastic drop of ductility leading to embrittlement. It has been shown recently that it is possible to add oxygen to a titanium alloy consisting of a binary Ti-Zr solid solution, to obtain the classical oxygen hardening contribution without any loss of ductility. The main objective of this postdoc is the accurate determination of the different phases existing in these new Ti-Zr-O alloys using thermodynamic modeling at the atomic scale and making use of ab initio calculations. We will in particular focus on the oxygen ordering tendency in titanium and on the impact of zirconium addition on this ordering, as the ductility loss induced by oxygen in titanium alloys is believed to be linked to the apparition of Ti_6O ordered compounds and/or to the development of short range order.

This postdoc is part of a project, ANR TiTol, involving four different French laboratories (IRCP Chimie ParisTech, ICMPE Univ. Paris Est, Diffabs Soleil and SRMP CEA Saclay). It will benefit from interactions with experimental work performed inside the project (alloy design, microstructural and mechanical characterization, synchrotron X-ray diffraction). In particular, predictions of the modeling approach will be directly compared to, but also guided by, X-ray diffraction experiments and resistivity recovery and calorimetry experiments

Laboratory: SRMP, laboratory of physical metallurgy, is part of CEA, the French atomic energy agency. The research center of Saclay is located 20 kilometers South of Paris to which it is connected by public transportation.
More information on CEA: http://www.cea.fr/english

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Time frame: The position is available immediately and the funding is for two years.

Qualification: The applicant should hold a Ph. D. Degree in solid state physics or materials science, with skills in one or more of the following simulation methods:

- Density functional theory
- Modeling of alloys thermodynamics

Experience in computer programming is also highly recommended.

How to apply: Candidates should send their application (statement of research interest, CV, names and contact information of two references) to emmanuel.clouet@cea.fr