Fiche de présentation
Formation Thématique ECOLE DOCTORALE 3MPL

Nom de la Formation Thématique : Computational Molecular Modeling of Materials and Interfaces (Lectures)

Code : 3MPL140

Etablissement dont relève la formation : EMN

UFR ou Ecole organisatrice : EMN

Localisation des enseignements : EMN

Capacité d'accueil : 15

Responsable : Nom : Kalinichev Prénom : Andrey Courriel : kalinich@subatech.in2p3.fr

Nombre de crédits ECTS : 4

Volume horaire pour l'étudiant : 12h (2 days)

Visioconférence possible : Oui

Compétences pré-requises : Basic knowledge of thermodynamics and physical chemistry. Basic quantitative and computer skills.

Compétences à acquérir par l'étudiant dans cette formation : 1) Understanding of the methods and techniques of classical molecular simulations (Monte Carlo and molecular dynamics); 2) How various properties of materials (structural, thermodynamic, kinetic, spectroscopic) can be calculated from such simulations and compared with experimental data; 3) Ability to qualitatively and quantitatively assess and analyze the results of such simulations published in the current research literature.

Modalités de validation de ces compétences :

Attendance

Résumé de la formation : The course introduces the methods and techniques of classical computational molecular modeling and their application to the fundamental understanding of the atomic- and molecular-level origins of physical and chemical properties of various inorganic and organic materials and processes related to many natural and engineeting applications.
The course is intended for students with relatively limited background in theoretical thermodynamics, statistical mechanics, molecular materials science, and computer programming, etc., essentially for those who are perhaps doing mainly experimental research, but who still need and desire to know and understand at least some basics of molecular modeling techniques in order to better understand modern approaches and current scientific literature on the subject relevant to their PhD projects

Informations complémentaires : The course is aimed at PhD students with little or no previous experience in molecular modeling. At present, the course can be offered only in English. The course consists of 2 parts: after the lecture part described above, a practical workshop can be taken which can help the students to use this knowledge for setting up and running simple molecular simulations of materials of their interest, and analyzing their results using existing software.