Fiche de présentation
Formation Thématique ECOLE DOCTORALE 3MPL

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

Code : 3MPL240

Etablissement dont relève la formation : EMN

UFR ou Ecole organisatrice : EMN

Localisation des enseignements : EMN

Capacité d'accueil : 5

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 : Non

Compétences pré-requises : Successfully completed first part of the course (Computational Molecular Modeling of Materials and Interfaces (Lectures)) is expected

Compétences à acquérir par l'étudiant dans cette formation : 1) Ability to set up and run simple classical molecular simulations of materials of their interest using existing software; 2) ability to qualitatively and quantitatively assess and interpret the results of such simulations

Modalités de validation de ces compétences :

Attendance

Résumé de la formation :

- building the molecular models of materials relevant to the student's PhD project
- selecting force fields for molecular simulations of materials
- using molecular mechanics, energy minimization and structure optimization techniques
- preparing input parameters for molecular dynamics simulations of the prepared models
- running short MD simulations of the prepared models (equilibration and production runs)
- analyzing and interpreting thermodynamic results of the simulations
- analyzing and interpreting structural results of MD simulations
- calculating the diffusion coefficients of the species present in the system
- using velocity autocorrelation functions to calculate and interpret power spectra of atomic motions relevant to the prepared models

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. This is the second (practical) part of the course, which can be taken after the theoretical (lecture) part. **:** The course is intended to be taught using the Materials Studio molecular simulations software package, and the course capacity (5 students) is currently limited by the number of available software licenses. The course capacity can be increased if more licenses are purchased or if the students will work not on their individual practical projects, but in teams of 2-3 persons.