



Post-doc position @ Institut Jean Lamour, Nancy, France

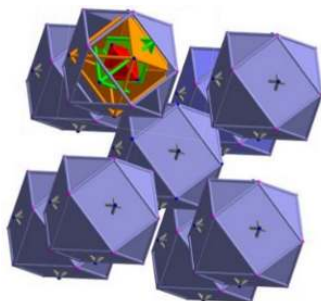
Ab-initio investigations of complex intermetallics surfaces : from structures to properties

Quasicrystals (QCs) are a novel class of solid materials with quasiperiodic translational symmetry and rotational symmetries forbidden in periodic crystals. Today, the field is very active, and QCs are being discovered in a broad range of systems. Hundreds of intermetallic compounds with quasiperiodic structures have been identified in phase diagrams. Soft QCs are an emerging field in colloidal and supramolecular chemistry. Perovskite oxide thin films with quasiperiodic structures have recently been identified, and even water thin films have been predicted to adopt quasiperiodic structures under specific conditions.

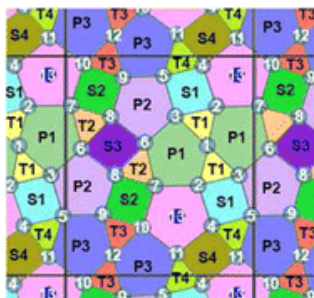
The research project will focus on intermetallic compounds with quasicrystalline structures and related phases. It includes periodic approximant, i.e. crystalline solids with similar chemical composition to a QC, but whose atomic arrangement is slightly distorted so that the symmetry conforms to the conventional laws of three-dimensional crystallography. Crystalline approximants can be considered the missing link between QCs and crystals and are very useful because they provide a well-defined starting point for models of the local atomic structure of the corresponding quasicrystals.

The purpose of the work is to understand and design complex intermetallic surfaces down to atomic and electronic scales, in relation to several potential applications (as catalysts or functional coatings, among others). Areas of interest include, but are not restricted to, electronic properties, computational catalysis, modeling of molecular films on intermetallic surfaces. Methods will be based on density functional theory and possible machine learning approaches, in collaboration with the neighboring research lab in computer sciences (Loria, Nancy).

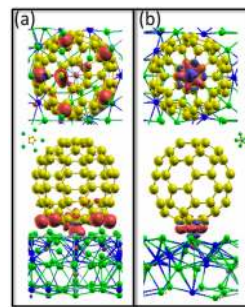
The activity is funded in the framework of a European FEDER project. It will take place in an international environment, involving several research networks : European consortium on complex metallic alloys (ECmetAC), International Associated Laboratory between IJL (Nancy, France) and JSI (Ljubljana, Slovenia), International Research Network between Japan, Germany and France. The Jean Lamour Institute is located on the campus Artem Nancy, gathering more than 5000 people including 3500 students.



Al_4Cu_9 bulk



$\text{Al}_{13}\text{Co}_4(100)$ surface



$\text{C}_{60}/i\text{-AlPdMn}$

The successful candidate will have a PhD degree in Chemistry, Physics, Materials Science, or a related field and deep knowledge in modeling. Programming experience, e. g. in python, are advantageous. A high degree of self-motivation, ability to work in an international team and to collaborate with computational and experimental colleagues, as well as good oral and written communication skills are expected.

The position is initially funded for 12 months (extendable to 24 months or more) and it will possibly start in September 2019. Interested applicants should send a cover letter, a curriculum vitae and the name of 2 referees to Émilie Gaudry: Emilie.Gaudry@univ-lorraine.fr