Séminaire

INSTITUT Charles SADRON
CNRS - UNISTRA - STRASBOURG

Mardi 20 février 2024 à 10h30

Amphithéâtre Henri Benoît

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Exploring the Atomic Landscape:
Molecular Modeling for Biomaterials Design

The emergence of biomaterials requires an understanding of the interactions between biomolecules and materials at the atomic scale. Faced with the challenges and difficulties of obtaining these experimental insights, molecular modeling stands out as an enticing approach to acquire such information at a reasonable cost. Furthermore, a detailed comprehension of interfaces through molecular modeling allows for the prediction of biomaterial behavior before its synthesis.

The field of modeling applied to biomaterials is still in its infancy, and numerous parameters need to be mastered. Nevertheless, one technique emerges amidst the complexity of systems and their intrinsic flexibility: molecular dynamics.This method not only offers a cost-effective means of gaining insights into atomic-scale interactions but also holds the potential to perform computer-aided biomaterials design in diverse applications.

In this context, I will illustrate the field of molecular modelling for biomaterials with several applications ranging from biosensors to biomaterials functionalized with biomolecules ranging from proteins to nucleic-acids.

Les personnes souhaitant rencontrer F. Barbaul sont priées de prendre contact avec Fouzia Boulmédais.