Toulouse, France,  
March, 24-26, 2014  

SIMULATION OF BIOMOLECULAR INTERACTIONS  
WITH INORGANIC AND ORGANIC SURFACES  
AS A CHALLENGE FOR FUTURE NANOTECHNOLOGIES

Symposium Organizers:  
Alain Estève, LAAS-CNRS, Toulouse, France  
Marie Brut, LAAS-CNRS, Toulouse, France  
Carlos Aleman, Universitat Politècnica de Catalunya, Spain  
Priya Vashishta, University of Southern California,
Monday, March 24th, 2014

8:50 – 9:00
Welcome from the organizers

Session 1: Modeling Issues in Bio-Hybrid Materials

9:00 – 10:10
Chairman: (to be confirmed)

09:00  Scale-bridging simulations at (bio)organic/mineral interfaces
       Christine Peter
       University of Konstanz, Germany

09:35  The role of hydrophobic surfaces in increasing recognition and binding
       affinity of amyloidogenic Josephin domains: a molecular modeling
       investigation
       Andrea Danani
       University of Applied Sciences of Southern Switzerland, Switzerland

10:10  Coffee break

Session 2: Peptide-Based Interfaces I (Inorganic)

10:40 – 12:25
Chairman: (to be confirmed)

10:40  Adsorption of biomolecules on metals and oxides from first principles
       Dominique Costa
       Chimie Paristech, France

11:15  Adsorption, diffusion and clustering of lysozyme at a charged ionic surface
       Paul Mulheran
       University of Strathclyde, Scotland

11:50  Investigating peptide adsorption selectivity using advanced molecular
       simulation
       Tiffany R. Walsh
       Deakin University, Australia
SESSION 3: PEPTIDE-BASED INTERFACES II (MEMBRANES)

14:00 – 15:30
chairman: (to be confirmed)

14:00  Tailoring Bio/Nano interfaces by mutagenesis: rational control of molecular interactions of peptides on solid surfaces
Mehmet Sarikaya
University of Washington, Seattle, USA

14:35  Molecular Dynamics simulations of short peptides: a useful tool to study versatile molecules
Gianfranco Bocchinfuso
Università di Roma Tor Vergata, Italy

15:10  Role of long-range protein-protein in the formation, stability and specialization of bio-membrane nano-domains
Nicolas Destainville
Toulouse University, France

15:45  Coffee break

SESSION 4: PEPTIDE-BASED INTERFACES III (NANO-OBJECTS)

15:45 – 17:30
chairman:

15:45  Monitoring the unfolding of soluble peptides at the sodium dodecyl sulfate micellar surface
G. Roussel, C. Michaux, Eric Perpete
University of Namur, Belgium

16:20  Robotics-inspired algorithms to explore energy landscapes
Juan Cortes
LAAS-CNRS, Toulouse, France

16:55  Atomistic simulations of protein-gold surfaces interaction for nanotechnologies
Stefano Corni
Docking of b2-microglobulin to gold nanoparticles
Giorgia Brancolini
Institute of nanoscience, Modena, Italy
Tuesday, March 25th, 2014

Session 5: General Perspectives from Theory/Experiment

9:00 – 10:10
Chairman:

09:00 Challenges for the molecular simulation of multi-phase biohybrid systems
Robert A. Latour
Clemson University, USA

09:35 Modelling of protein adsorption on solid surfaces using brownian and molecular Dynamics simulations
D.B. Kokh, J. Romanowska, M. Ozboyaci, R.C. Wade
University of Heilderberg, Germany

10:10 Coffee break

Session 6: DNA-based Interfaces I

25 March, 9:00 – 11:10
Chairman:

10:40 Meeting Materials challenges in nanopore sequencing of DNA
Aleksei Aksimentiev
University of Illinois, USA

11:15 DNA sensing based on modified diamond-like nanostructures
Maria Fyta
University of Stuttgart, Germany

Session 7: General Discussion and Poster Session

11:15 – 12:30

14:00-19:00: Free

20:00-23:00: Social Dinner
SESSION 7: DNA-BASED INTERFACES II

9:00 – 11:10
chairman:

9:00  Programming matter with DNA
Anthony Genot
LIMMS/CNRS-Institute of Industrial Science, University of Tokyo, Japan

9:35  DNA interactions with surfaces of interest in nanotechnologies: a first principle study
Anne Hemeryck
LAAS-CNRS, Toulouse, France

10:10  coffee break

SESSION 8: DNA-BASED INTERFACES III

10:40 – 11:50
chairman:

10:40  Interaction of DNA with Hydroxyapatite: surface adsorption and biomineralization
Carlos Aleman, Pau Turon, Jordi Puiggali
Universitat Politecnica de Catalunya, B. Braun Surgical S.A., Spain

11:15  Structural Behaviours of Cytosine into the hydrated interlayer of Na+-Montmorillonite clay: an ab initio Molecular Dynamics study
Pierre Mignon
Université de Lyon, UMR 5280 Villeurbanne, France

11:50  Petascale simulations of aqueous clay-mineral interfaces
Peter V. Coveney, Sofia Shamin
University College of London, UK