5th CCPBioSim/CCP5 Multiscale Modelling Conference

Programme

Day 1 - Monday 3rd April 2023

12:00 – 13:20	**Registration and Lunch**
13:20 – 13:30	Welcome / Introduction
13:30 – 14:05	Rosana Collepardo *Title*
14:05 – 14:25	Daniel Del Hoyo *Scipion-chem: an Open Platform for Virtual Drug Screening*
14:25 – 14:45	Mark Driver *Protein-RNA Condensates: Complementary or Competing Interactions in ALS Progression?*
14:45 – 15:15	**Coffee Break**
15:15 – 15:50	Modesto Orozco *Advances and challenges in the simulation of DNA*
15:50 – 16:10	Giulia Frigerio *Molecular Dynamics Simulations of cRGD-conjugated PEGylated TiO2 Nanoparticles for Targeted Photodynamic Therapy*
16:10 – 17:00	*Flash Talks A – Odd Poster Numbers*
17:00 – 18:30	**Poster Session A**

Day 2 - Tuesday 4th April 2023

08:30 – 09:00	**Welcome**
09:00 – 09:35	Björn Baumeier *Theoretical Spectroscopy of Complex Multiscale Materials with Embedded Green's Function Methods*
09:35 – 09:55	Lianne Gahan *Coarse Grained Modelling of Amyloid Fibril Formation, Inhibition and Disruption Towards Alzheimer's Drug Design*
09:55 – 10:15	Marko Hanzevacki *Multiscale Modelling of Reactions in Radical Metalloenzymes*
10:15 – 10:35	Rachel Hendrikse *Using Many-body Dissipative Particle Dynamics to Predict the Surface Tension of Pure and Mixed Systems*
10:35 – 11:05	**Coffee Break**
11:05 – 11:40	Paola Carbone *Modelling the structure of the carbon/electrolyte interface using QM/MD simulations and machine learning*

11:40 – 12:00	Victoria Hill *DNA Damage Competes With Sequence to Pin a Plectoneme*
12:00 – 13:30	**Lunch Break**
13:30 – 14:05	Halim Kusumaatmaja *Wetting of Biomolecular Condensates in Biological Cells*
14:05 – 14:25	Jaehyeok Jin *Systematic Design Principles for Combining Rules in Bottom-up Coarse-Grained Interactions*
14:25 – 14:45	James Krieger *Scipion-EM-ProDy: A Graphical Interface for the ProDy Python Package enabling Integration of Databases, Simulations and Cryo-Electron Microscopy Image Processing*
14:45 – 15:15	**Coffee Break**
15:15 – 15:50	Laura Orellana *Connecting Biological Scales – From Disease Mutations to Protein Mechanisms Through Coarse-grained and Atomistic Simulations*
15:50 – 16:10	Tomas Kubar *Simulation of Reactions in Biomolecular Complexes: Blending the Flavours*
16:10 – 17:00	*Flash Talks B – Even Poster Numbers*
17:00 – 18:30	**Poster Session B**
19:00	**Conference Dinner**

Day 3 - Wednesday 5th April 2023

08:30 – 09:00	**Welcome**
09:00 – 09:35	Cecilia Clementi *Title*
09:35 – 09:55	Andrea Levy *Free Energy Profiles of Transition Metal Drug Binding From Multilevel Thermodynamic Integration*
09:55 – 10:15	Antoni Salom Català *Computational Modelling of Gas-Liquid Pickering Interfacial Catalysts Using Dissipative Particle Dynamics*
10:15 – 10:35	Sergio Sousa *Application of QM/MM Methods to Understand the Role Played by Different Amino Acid Residues in the Catalytic Mechanism of Plastic PET degrading Enzymes*
10:35 – 11:05	**Coffee Break**
11:05 – 11:25	Tseden Taddese *Mesoscale Modelling and Simulation of Water/poly(ethylene oxide) on Silica Surfaces*
11:25 – 11:45	Stephen Yeandel *Interfacial Free Energies from MD Simulations: Application to CaSO4.xH2O*

11:45 – 12:20	Matteo Salvalaglio *Nucleation of Biomolecular Condensates from Simulations and Experiments in Finite-Size Volumes*
12:20 – 14:00	**Lunch and Close**

Posters

Number	Presenter	Title
1	Ahmed, Saleh Hussein Abduraboh	Structural Properties and Insights of Water-methanol Mixtures – An Atomistic Molecular Dynamics Simulations Study
2	Boeser, Julian	Reduction Pathway of Glutaredoxin 1 Investigated with QM/MM Molecular Dynamics Using a Neural Network Correction
3	Chao, Kin	A Multiscale Simulation Approach to Characterise the Glidesome-associated Connector (GAC) from Toxoplasma gondii
4	Chen, Zhongquan	Multiscale Modelling of Charge Dynamics in Neuromorphic Devices
5	Chergui, Yahia	Measurement of ZnO Atomic Distances under Isothermal and Isobaric Ensembles: A Molecular Dynamics Prediction
6	Eichinger, Lena	Exploring the Mechanism of Autophosphorylation in the Bacterial Sensory System using QM/MM Simulations
7	El-Sayed, Sherihan	Insights into NLRP3 Inflammasome Activation Using MD Simulation
8	Fan, Lanyu	Study of Monoclonal Antibody Formulations to Decrease Aggregation Using Molecular Simulations
9	Farouq, Haider	Adsorption of The Spike Protein On a Model Silica Surface
10	Ferguson, George	Investigating the Intercalation of Cryptolepine between DNA Watson and Crick Base Pairs
11	Gonçalves de Abrantes, Juliana	Quantum Tunnelling in Methylated DNA
12	Güven, Jasmin	Potential Inhibitors for Beta-lactamases Under the Alchemical Microscope
13	Hoffmann, David	Exciton Transfer Simulations in Light Harvesting Complexes Accelerated by Machine Learning
14	Hori, Naoto	Mg2+-induced Folding and Misfolding of Ribozyme Studied by

		Coarse-grained RNA Model
15	Huertas, Jan	The Pioneer Transcription Factor Oct4 Alters Chromatin Packing
16	Iorio, Antonio	Multiscale Shear Flow Induced Aggregation of Aβ Amyloid in Interstitial Brain Space
17	Kanagarajan, Ajeeth	Studying the Permeation of Small Molecules in Poly Vinyl Acetate, PVAc
18	Laborie, Emeline	Towards a Realistic Multiscale Model of Cilia Driven Clearance
19	Lightfoot, Jasmine	Understanding the Improved Separation Performance of Asymmetric Polymer Composite Membranes
20	Maristany, Maria Julia	Mechanistic Properties of DNA Govern Nucleosome Unwrapping
21	Morbec, Juliana	Pentacene Molecules Meet Transition Metal Dichalcogenides for Photovoltaic Energy Harvesting
22	Musleh, Sondos	Absolute Binding Free Energy Calculations of Monosaccharide and Oligosaccharide Ligands of Concanavalin A
23	Nesabi, Azam	Predicting the Aggregation of Small Molecules by Molecular Dynamics Simulation
24	Ngambia, Audrey	Molecular Models of Realistic Biochars with Controlled Porosity
25	Robins, James	Development of Coarse-grained Molecular Simulation Model for Polymer-RNA Nanoparticles
26	Slocombe, Louie	Quantum Tunnelling Effects in the Guanine-Thymine Wobble Misincorporation via Tautomerism
27	Spies, Katharina	CP-DFTB/MM Simulations of Tyrosine-tyrosine PCET in RNR-Inspired Model Systems
28	Stavert, Tom	Modelling-Assisted Development of Green Routes to Ordered Mesoporous Silica
29	Stennett, Amelia	Turning up the Heat: Understanding of the Sensitivity of NLRP3 Inflammasome to Elevated Temperature
30	Trnka, Tomáš	Efficient Pipe Interface Between the Amsterdam Modeling Suite and External Software
31	Vallee, Cedric	Investigation of Heavy Water Effect on Ion Selectivity in ASIC1
32	van Vuren, Oscar	Developing Standardised Modelling Workflows for Multiscale QM/MM Studies of Metal Oxides

33	Vu, Huong	Plus and Minus Ends of Microtubules Respond Asymmetrically to Kinesin Binding by a Long-range Directionally Driven Allosteric Mechanism
34	Walsworth, Sam	Cytotoxic Ag-NHC Complexes as LDHA Inhibitors
35	Wang, Yuhan	Using Molecular Dynamics Simulation to Predict the Aggregation Propensity of Monoclonal Antibodies Formulations & Accelerate Development
36	Winokan, Max	The Replisome Environment and DNA Point Mutations: Multiscale Simulations of G-C Tautomerism and PcrA Helicase
37	Xu, Shangze	Mechanistic Investigation of the Androgen Receptor DNA-Binding Domain and Modulation via Direct Interactions with DNA Abasic Sites: Understanding the Mechanisms Involved in Castration-Resistant Prostate Cancer
38	Zaki, Afroditi Maria	Binding and Mode of Action of the Ectoparasite Fluralaner to the GABA RDL Receptor of Insects