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Using a simple electrostatic model to study the interaction between proteins and surfaces

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Introduction, prof. **Guido Raos** (Politecnico di Milano, DCMIC)

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Room Natta, Bulding 6
Piazza Leonardo da Vinci, 32 Milano

live | online

link will be emailed to
registered participants

Registration Form

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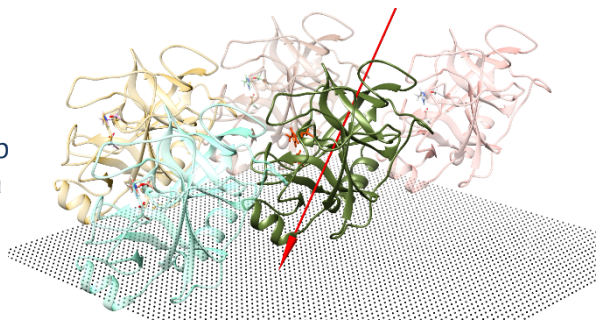

The interaction of proteins and surfaces is key for many biotechnological applications, including from biosensors, bioleaching, and catalytic surface design. Understanding these complex interactions, where electrostatics plays a major role, is of great interest. In this work, we used a simp electrostatic model to study how a protein interacts with a surface, which gives remarkable insights of the underlying physics. Our model uses the Poisson-Boltzmann equation To compute free energies, enabling the determination of the probability of different protein-surface configurations. Furthermore, we extended our study to explore the influence of electric fields to control the orientation of the proteins upon adsorption, showcasing great potential for fine-tuning the catalytic activity of the surface, even when the material was hydrophobic. During this presentation, we will discuss some implementation details of our numerical model, highlight its advantages and limitations, and provide future perspectives for broadening its application across other domains.

Dr. Christopher Cooper is an Assistant Professor at the Mechanical Engineering Department of Universidad Técnica Federico Santa María (USM) in Valparaíso, Chile. He obtained his undergraduate degree from USM in 2009 and went on to complete his MS (2012) and PhD (2015) degrees in Mechanical Engineering at Boston University. Leading a research group at USM, Dr. Cooper specializes in numerical modeling of molecular systems, with a particular emphasis on electrostatic simulations using partial differential equation models solved with the boundary element method. He is particularly dedicated to delivering these models in fast, accurate, and robust computational tools that are user-friendly and accessible to the wider scientific community.