Workshop - Immobilizing peptides and proteins: Interplay between theoretical and experimental approaches

Start Time: Tuesday, August 30, 2022

End Time:

UniSysCat group leader Prof. Maria Andrea Mroginski is co-organizing a CECAM-Workshop on "Immobilizing peptides and proteins: Interplay between theoretical and experimental approaches". There are still slots for Postdocs and PhD students available.

CECAM is the Centre Européen de Calcul Atomique et Moléculaire, an iInstitute for the promotion of fundamental research on advanced computational methods and their application to problems in frontier areas of science and technology.

The workshop - that's what it's about

When? October 4, 2022 - October 7, 2022
Where? CECAM-FR-MOSER, Institut de Biologie Physico-Chimique, Paris
Website for registration: www.cecam.org/workshop-details/1132
Organisers:

- Florent Barbault (University Paris Diderot)
- Maria Andrea Mroginski (Technical University of Berlin)
- Sophie Sacquin-Mora (Laboratoire de Biochimie Théorique, CNRS UPR9080)

The immobilization of peptides and proteins on membranes and solid supports has attracted growing interest in the biomaterials field over the last forty years, as this phenomenon plays a central part in numerous applications. When investigating the interaction between a biomolecule and a surface, two key issues that should be addressed are the stability of the interface, and the biomolecule orientation on this surface. For example, in bioelectrocatalysis devices it is essential to ensure correct protein orientation enabling direct electron transfer between the adsorbed redox enzyme and the electrode. In addition, one must make sure that

the enzyme active site remains accessible after immobilization. This can be achieved through targeted chemical linkage between the protein and the surface, or via the adequate functionalization of the surface. One must also pay attention to the conservation of the adsorbed protein's structure and dynamics, as perturbations in the protein conformation or internal mobility are likely to result in a dramatic decrease of the catalytic activity. These questions are especially important for devices such as biosensors or biofuel cells, which use redox enzymes grafted on functionalized surfaces, and therefore rely on the conservation of biomolecular function out of the cellular environment

Over the last decades, computational models have been playing an increasingly important part in this field, as they can bring greater hindsight on the chemical and biological processes taking place at the bionanointerface. The last decade has seen a wealth of methodological developments, in particular with empirical force fields parametrization for a wide range of materials, and multiscale approaches combining all-atom and coarse-grained representations. As a consequence, molecular simulations techniques are now a powerful tool in the biomaterials field. Simulations can provide us with information regarding the orientation of the adsorbed molecules, the strength of this absorption and its impact on their structure. This is of particular interest, since an important issue that has to be addressed when dealing with immobilized systems is the conservation of their reactivity. Recent work has shown that when setting up an immobilization strategy, one must achieve a delicate balance between the enzyme stability and its catalytic activity.

References

[1] A. Klibanov, Analytical Biochemistry, **93**, 1-25 (1979)
[2] R. Sheldon, S. van Pelt, Chem. Soc. Rev., **42**, 6223-6235 (2013)
[3] V. Hitaishi, R. Clement, N. Bourassin, M. Baaden, A. De Poulpiquet, S. Sacquin-Mora, A. Ciaccafava, E. Lojou, Catalysts, **8**, 192 (2018)
[4] M. Ozboyaci, D. Kokh, S. Corni, R. Wade, Quart. Rev. Biophys., **49**, e4 (2016)
[5] S. Dasetty, P. Meza-Morales, R. Getman, S. Sarupria, Current Opinion in Chemical Engineering, **23**, 138-145 (2019)
[6] J. Weltz, D. Kienle, D. Schwartz, J. Kaar, J. Am. Chem. Soc., **142**, 3463-3471 (2020)
[7] H. Xia, N. Li, X. Zhong, Y. Jiang, Front. Bioeng. Biotechnol., **8**, (2020)
[8] C. Marsh, G. Shearer, B. Knight, J. Paul-Taylor, A. Burrows, Coordination Chemistry Reviews, **439**, 213928 (2021)