Peptides at Surfaces:
Simulating Organic-Inorganic Interface Systems

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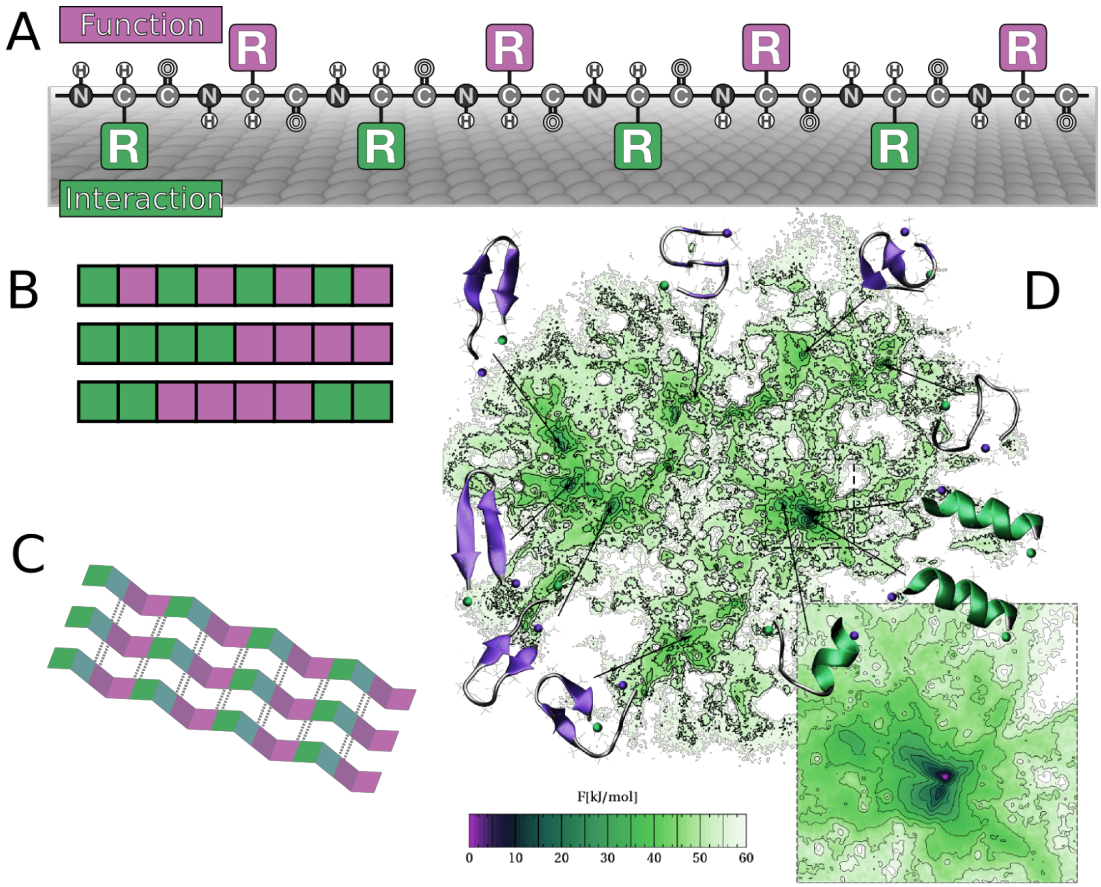

The combination of the virtually infinite chemical space of peptides with the well defined characteristics of surfaces opens routes to multiple applications ranging from detailed structural characterization, to coated implants for sensors in medicinal diagnostics, and supported bio-catalysts. In close collaboration with the experimental team of Dr. Rauschenbach at MPI Stuttgart, this project will investigate from a modelling perspective the determinant factors for the structure and dynamics of peptides in contact with inorganic surfaces. To accomplish that, we will develop methods to describe and investigate these interactions, combining the accuracy of first-principles electronic structure theory and the time and size scales needed to account for entropic effects. In order to study the interactions between the surface and the peptides with predictive accuracy it is mandatory to design new empirical models based on electronic structure calculations. The prediction of structure formation has to consider: (i) peptide conformation, (ii) peptide-surface interaction, and eventually (iii) peptide-peptide interaction at the surface. Machine-learning techniques will assist the analysis of the complex conformational landscape and accelerate its exploration.

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[2] Chen, J.; Edwards, S. A.; Gräter, F.; Baldauf, C.;J. Phys. Chem. B 31 (2012): 9346
[3] Rossi, Mariana, Matthias Scheffler, and Volker Blum. The Journal of Physical Chemistry B 117 (2013): 5574.