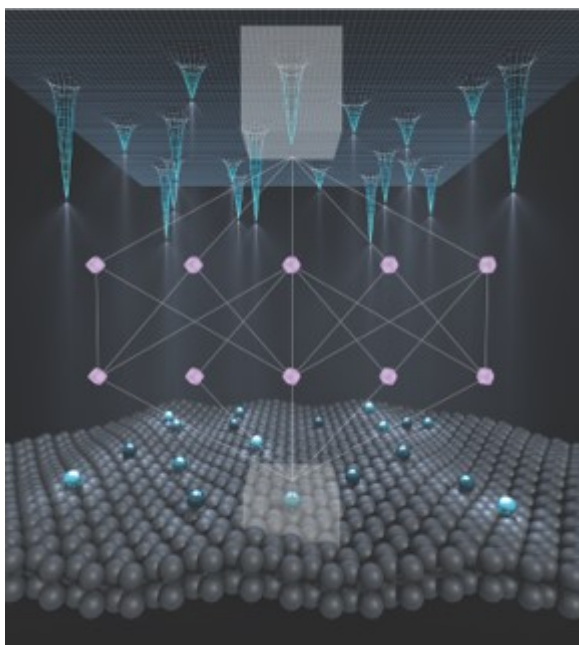


Hybrid SORS/WiCS: Sustainable chemistry and catalysis design meet digitalization

Objectives

Abstract: Catalysts play a critical role in directing and accelerating the conversion of reagents into targeted products. The design of novel and/or improved catalysts is central to enable the sustainable production of fuels and value-added chemicals. This is a crucial challenge that requires a multi-disciplinary approach, and in turn, it will help address the complex socio-economic and environmental issues of our time. In this talk we will introduce the challenges of developing improved catalytic processes, and the importance of large collaborative initiatives, such as NCCR Catalysis, a Swiss National Center of Competences in Research. Next, we will discuss the role of computational modeling, high performance computing, and machine learning, in advancing catalysis design. In particular, we will showcase two collaborative research projects where deep learning methods and quantum chemistry simulations are exploited to characterize the structure of low nuclearity catalysts, an emergent class of materials uniquely positioned to enable sustainable catalytic conversion processes.



Short bio: The talk will be presented by an international and

multidisciplinary team of scientists from the Advanced Catalysis Engineering Laboratory at ETH Zurich, the Institut Català d'Investigació Química, and the Barcelona Supercomputing Center. The team expertise spans from microscopy to computational modeling, through catalysis engineering and machine learning. Their research activity develops in the framework of the NCCR Catalysis, whose vision is to establish Switzerland as an internationally-recognized center for sustainable chemistry research, education, and innovation.

Speakers

Speakers: K. Rossi¹, A. Ruiz-Ferrando², S. Mitchell¹

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Host: Dario Garcia Gasulla, Artificial Intelligence Associated Researcher, Computer Sciences

Barcelona Supercomputing Center - Centro Nacional de Supercomputación

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