Prospects and challenges for computer simulations of monolayer-protected metal clusters and their aggregates

Monolayer-protected clusters (MPCs) have a monometallic or intermetallic core that is stabilized by an organic ligand layer. They form a novel class of atom-precise nanomaterials with tunable properties for possible applications, e.g., in catalysis, biological sensing, biological imaging, and in nanomedicine. The vastly increasing data on their atomic structure from single-crystal X-ray diffraction experiments creates input for atomistic simulations to understand their chemical, physical, and bio-compatible properties. In this talk, I will discuss the challenges in modeling MPCs at various levels of accuracy suitable for needed size- and time-scales, coupled with the need to understand their interactions with the environment. The palette of simulation methods is based on both quantum and classical physics, and I will show select recent case studies prompted by collaborations with experiments. The talk is concluded with discussion of the rising prospects of data-driven machine learning.

CARBON TO METAL COATING INSTITUTE
at Queen's University

Seminar

Prospects and Challenges for Computer Simulations of Monolayer-Protected Metal Clusters and Their Aggregates

Dr. Hannu Häkkinen

University of Jyväskylä
Finland

24 MAY 2022 | **11:30 AM 12:30PM** | **Room CHE 117**

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