# O 84: Key Note VI

Time: Wednesday 15:30–16:00 Location: R1

**Plenary Talk** O 84.1 Wed 15:30 R1

**Surface structure by way of machine learning** — •Bjørk Hammer — Aarhus University, Denmark

Atomistic simulations of the physico-chemical processes at inorganic surfaces often require knowledge of the energetically most optimal state of the surfaces. In this talk, examples are given of intricate surface reconstructions and surprising shapes assumed by metal nanoparticles supported on oxide surfaces. The focus of the talk will be on how to identify such optimal structure given a costly total energy method as implemented in an electronic structure program, typically a density functional theory program (DFT). A number of approaches will be presented. i) A purely **evolutionary approach**[1] in which new structural candidates are created by random cross-over and mutation operations, ii) a **machine learned-enhanced evolutionary approach**[2,3] in which an on-the-fly learned surrogate energy landscape directs the candidate production, and finally iii) a **reinforcement learning approach**[4] in which image recognition via a convolutional neural network is used to build up rational knowledge about the energy landscape, that eventually leads to the construction of globally optimal structure.

[1] Phys. Rev. Lett. **108**, 126101 (2012).
[2] Phys. Rev. Lett. **124**, 086102 (2020).
[3] **https://gofee.au.dk**
[4] Phys. Rev. B, **102**, 075427 (2020).