O 37: Overview Talk: Bjørk Hammer

Time: Tuesday 9:30–10:15 Location: TRE Phy

Topical Talk O 37.1 Tue 9:30 TRE Phy

Automating computational surface structure determination — •Bjørk Hammer — Aarhus University, Denmark

Accurate models of surface structure are required whether rationalising experimental observations or providing theoretical predictions. In recent years, density functional theory (DFT) investigations have matured to a level where thousands of computations may be conducted in a reasonable time frame. This has opened up for automating the search for structure of the outermost layers or nano-scale agglomerates at surfaces. For few-dimensional problems, such as the structure of molecular adlayers, grid searches provide a reliable means for finding the global minimum energy structure. For higher-dimensional problems, such as entire surface structures or surface supported nano-particles, a stochastic approach toward identifying the global minimum energy structures may be adopted. Here, evolutionary algorithms (EAs) have proven succesful. In the talk, various ways of enhancing the success of EAs with machine learning and big data methods will be demonstrated. As EAs methods remain stochastic in nature, there is no buildup of knowledge that can be transferred from one EA run to the next. The talk will outline how image recognition and reinforcement learning techniques [1] may remedy this and help building artificially intelligent learning system that may transfer knowledge from solving one surface structure problem to the next.

[1] See: https://asla.au.dk