Aalto University

Dissertation press release **10.09.2020**

The needle in the nanostack – Computational screening of catalysts

Title of the dissertation	Efficient screening of nanoclusters as catalysts for the hydrogen evolution reaction
Contents of the dissertation	Catalyzing the splitting of water is an important reaction for energy storage applications. Catalysts at the order of a few nanometers have different properties and have the potential to outperform existing ones. Computer simulations enable the design of a new catalyst from scratch. However, the design of new catalysts via such simulations requires enormous time due to the vast space of catalysts combination. This dissertation addresses the screening of nanoclusters and proposes new sampling techniques, adsorption site classification methods and leverages the power of machine learning to save computation time. A program is presented which automates the production of large datasets of simulations. This tool will help to speed up the discovery of potentially cheaper and better catalysts.
Field of the dissertation	Physics Engineering
Doctoral candidate	Marc Jäger, MSc
Time of the defence	30.09.2020 at 11:00
Place of the defence	Remote connection zoom under the link https://aalto.zoom.us/j/61477725193
Opponent	Professor Thomas Bligaard., Technical University of Denmark, Denmark
Custos	Professor Adam Foster, Aalto University School of Science, Department of Applied Physics
Electronic dissertation	
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