POLiS
Post Lithium Storage
Cluster of Excellence

POLiS Seminar Series – 20 September 2023

Rational design of new electrocatalytic materials for energy and sustainability

Hannah-Noa Barad
Department of Chemistry, Center of Nanotechnology & Advanced Materials,
Bar Ilan University, Ramat Gan, Israel
hannah-noa.barad@biu.ac.il

Abstract

Discovery of new, stable, and highly active catalyst materials is a pressing issue as part of trying to mitigate global climate change and improve sustainable resources. Currently the most efficient and stable catalysts for the chemical processes that we use to transform raw resources into products with desired functions (chemicals or energy), e.g., H2 evolution and CO2 reduction, contain expensive rare and precious elements such as Pt and Ir. This explains the efforts to find abundant, accessible, low-cost, stable alternatives that will yield process efficiencies comparable or better than those we have today. For example, for water split-ting, many new materials with different compositions have shown promising results as catalysts. However, they are mostly prepared by wet chemical synthesis, which results in chemical waste and can be too slow for industrial use. Second, the morphology of the catalysts is important because it affects their catalytic properties as higher surface areas yield more catalytically active sites, surface energetics change, etc. These reasons emphasize the motivation to accelerate the process of finding new materials with varying nanostruc-tures and optimized functionality, by systematic exploration of several parameter spaces

In recent years, artificial intelligence, namely machine learning (ML), has advanced within the field of materials science. The use of ML accelerates new material predictions and assists with finding unexpected correlations between the process-structure-function relations of materials. This leads to a better understand-ing and focus of the vast parameter spaces that exist in materials science. Rational design by ML in con-junction with combinatorial materials science promotes the rapid discovery and analysis of new materials, and enables breakthroughs in materials science, which are otherwise not possible.

Here I present the progress in the development of electrocatalysts using rational design with ML in con-junction with combinatorial synthesis and high-throughput characterization. We investigate changes in composition and nano-morphology on material libraries and their effects on the electrocatalysis of reactions such as O2 evolution, CO2 reduction, and CH3OH oxidation.

The different nanostructures and compositions show high activity and stability as electrocatalysts. The insights gained herein, indicate a dependence of catalytic activity on composition and nanostructuring, which the standard experimental techniques cannot achieve or explore, illustrating the importance and impact that composition and structure have, and will have, on developing sustainable catalysts. This can only be done by high-throughput experimentation de-sign, combined with machine learning tools, which will assist with appropriate path directions and ensure rational studies on catalysts in the future.