Type of report

GCS popular science report

Project title

Tailoring transition metal oxide catalysts for the oxygen evolution reaction via data-driven descriptor engineering

HPC System(s) and corresponding centre(s)

JUWELS Cluster of the Jülich Supercomputing Centre

Project ID

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Learning the binding of complex molecules to catalyst surfaces

The way how molecules involved in chemical reactions bind to the surface of a catalyst is key to understanding and improving the catalyst's performance. Researchers from the University of Aarhus and the Fritz Haber Institute have now developed a machine learning algorithm that can predict this important property for complex molecules that can bind to the surface in multiple motives.

Do you like to play Tetris? In particular, at higher levels, when you have to quickly move the complex-shaped pieces into the best position? In some sense, computational catalysis researchers repeatedly have to excel in such a task. A key quantity they regularly compute with advanced quantum mechanical simulation software is how strongly a molecule binds to the surface of a potential catalyst material. The importance of this information was already discovered by Nobel laureate Paul Sabatier about a hundred years ago: If the binding is too weak, the molecule is not activated enough to efficiently engage in the catalytic reaction. If the binding is too strong, it has no further incentive to engage in the catalytic reaction and will simply block the catalyst surface.

Quantum mechanical calculations can reliably provide this important information, and this is increasingly used to assess the suitability of new catalyst materials before actually initiating the laborious task of synthesizing these materials in the laboratory. Unfortunately, the demanding calculations require supercomputers and just like in Tetris (see Figure 1), there are different positions on the surface to which the molecule could bind. By trying out all positions, each involving a new calculation, the researchers have to determine where the molecule fits best. Larger, complex molecules can furthermore bind in different ways and orientations to these positions, again, just like a complex-shaped piece in Tetris. With typically dozens of molecules involved in important catalytic reactions like the Fischer-Tropsch reaction to create synthetic fuels, it simply takes too long to perform the total number of required calculations. Game over.

An experienced Tetris player develops a feeling of where to best place the pieces. "Machine learning algorithms work analogously", explains Wenbin Xu, a Ph.D. student at the Fritz Haber Institute. Having been trained with the results of previous calculations for similar molecules and catalyst surfaces, these algorithms can make reliable predictions about the binding without the need for any further supercomputing time and thus much faster. Not surprisingly, with the advent of AI, the development of corresponding algorithms has become a hot topic. Up to now, however, existing algorithms could not properly cope with complex molecules. They could only predict the binding of small molecules that bind with one obvious orientation to the surface – just like a simple quadratic Tetris piece. "The missing information for the algorithms was the connectivity within the molecule. Which atom binds to which…", says Prof. Mie Andersen from the University of Aarhus. Relying on mathematical graph theory, the research team now found a way to provide this information. Their new machine-learning algorithm, published in Nature Computational Science, already provides accurate binding information for larger molecules that are centrally involved in Fischer-Tropsch and other important fuel generating reactions. Catalyst researchers have a new powerful Tetris player at their side.

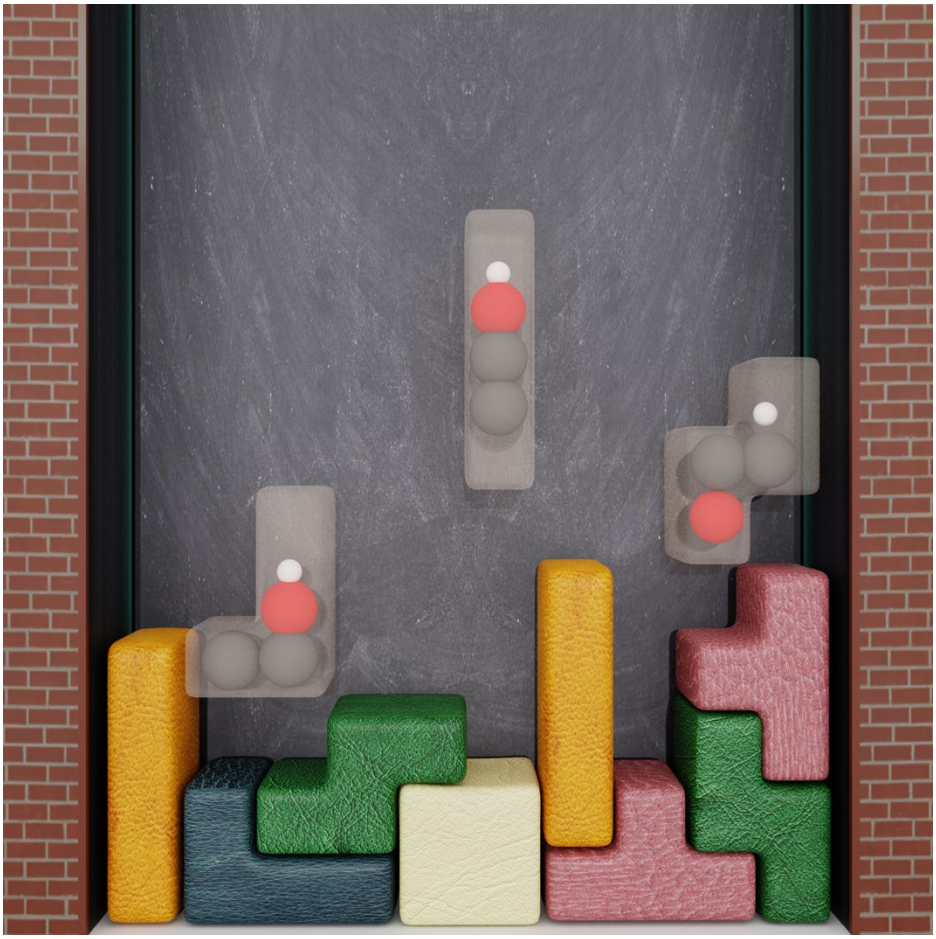

Figure 1. A machine learning algorithm predicts the binding of molecules to a catalyst surface. Reprinted with the permission from Copyright © 2022, Wenbin Xu, Karsten Reuter and Mie Andersen, under exclusive licence to Springer Nature America, Inc.

References:

W. Xu, K. Reuter, and M. Andersen. Predicting binding motifs of complex adsorbates using machine learning with a physics-inspired graph representation. Nat. Comput. Sci. 2, 443450 (2022).