Contribution ID: **39** Type: **Talk**

AI-driven discovery of material ”genes”: application to CO2 activation on semiconductor oxide surfaces (12 min talk + 3 min discussion)

Wednesday, 14 April 2021 14:30 (15 minutes)

Using subgroup discovery (SGD), an AI approach that discovers statistically exceptional subgroups in a dataset, we develop a strategy for a rational design of catalytic materials. SGD allows for the identification of distinct, possibly competing mechanisms of a catalytic activation. Here, it is applied to the problem of converting CO_2 into useful chemicals. We demonstrate that the bending of CO_2, previously proposed as the indicator of activation, is insufficient to account for the good catalytic performance of experimentally characterized oxide surfaces. Instead, our approach identifies the asymmetric strong elongation of the molecular C-O bond as a more accurate indicator.

Poster title

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