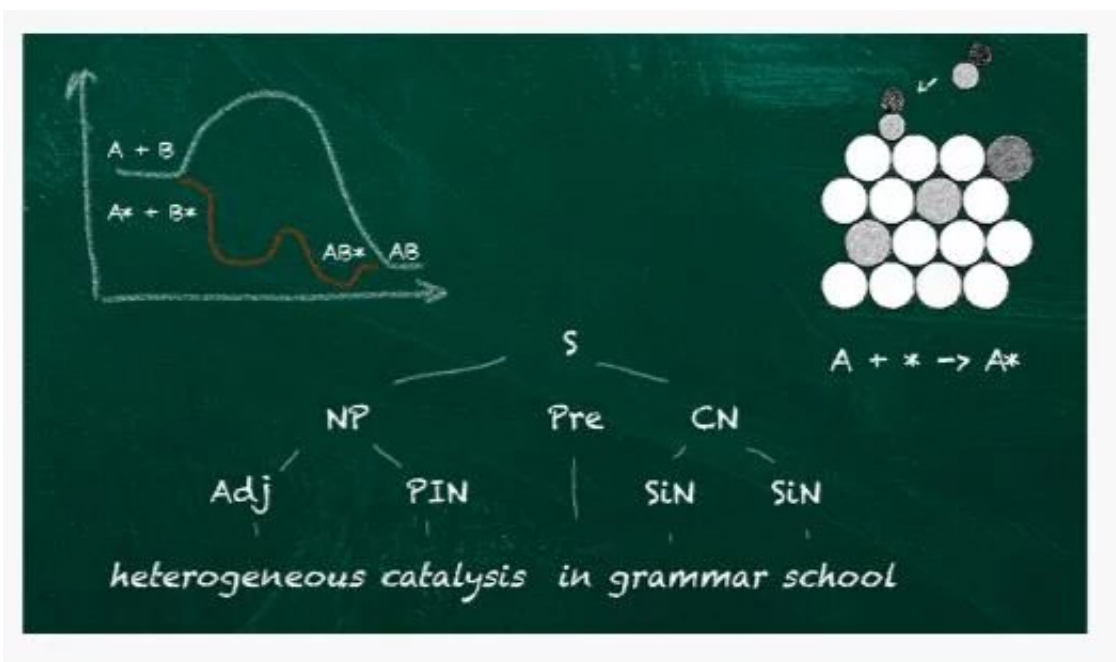


Searching for a grammar of materials to aid in discovery of catalysts

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Can new catalysts be discovered through formal grammars? Credit: Margraf et al

A research group from the Theory Department has explored the use of formal grammars as a new approach to discovering solid catalysts. Such grammars can encode the building rules of known materials and subsequently propose unknown materials with similar properties. By using the concept from computational linguistics, the Berlin-based scientists collaborated with US-American and South-Korean colleagues.

The discovery of new catalytically active materials is of great importance for accelerating the introduction of renewable energy sources and reducing the energy consumption of chemical industry. This search is highly challenging because catalysts have to fulfill a wide range of conditions like high activity, elemental abundance, low toxicity, long-term stability. At the same time there is a practically infinite number of materials that could potentially be interesting. The [grammar](#)-based approach proposed in this paper develops systematic building rules based on physical insight or known materials. These rules then allow the targeted generation of promising candidates, as demonstrated for simple ionic materials.

While this initial success is promising, it is clear that there is still a long way to go towards a grammar for heterogeneous catalysis. Real catalysts are complex structures that adapt dynamically under operating conditions. Finding grammatical production rules that capture this complexity is far from trivial. The researchers outline several potential paths to this goal, such as the inference of grammars from data using artificial intelligence.

More information: Johannes T. Margraf et al, Heterogeneous Catalysis in Grammar School, *The Journal of Physical Chemistry C* (2022). [DOI: 10.1021/acs.jpcc.1c10285](https://doi.org/10.1021/acs.jpcc.1c10285)

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