PAUL SCHERRER INSTITUT

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PSI Colloquium

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Fourth Paradigm of Materials Science: Novel Research Routes by Artificial Intelligence

Abstract

High-throughput screening of materials provides important, urgently needed information. However, as the number of possible materials is practically infinite, the amount of directly computed or measured information will always remain marginal. In this talk I will address this challenge in terms of “the fourth paradigm of materials research”, i.e. by artificial intelligence (AI) concepts that enable the identification of correlations and structure in the available big data of materials and to create ‘maps of materials properties’.[1,2]

Importantly, from the practically infinite number of materials, only about 10 of them may be relevant for a certain purpose. In simple words, in materials science and engineering, we are often looking for “needles in a hay stack”. Fitting or machine-learning all available data with a single, global model means fitting the hay, where one may average away the specialties of the interesting minority -- the needles. I will discuss methods that identify statistically exceptional subgroups[3] in a large amount of data, and I will demonstrate this for catalytic CO_2 activation (turning a greenhouse gas into fuels and useful chemicals).[4] Furthermore, I will discuss ‘a map for topological insulators’ as a class of quantum materials.

1) C. Draxl and M. Scheffler, *Big-Data-Driven Materials Science and its FAIR Data Infrastructure.* In Handbook of Materials Modeling (eds. S. Yip and W. Andreoni), Springer (2019).

2) R. Ouyang, S. Curtarolo, E. Ahmetcik, M. Scheffler, and L.M. Ghiringhelli, *SISSO: a compressed-sensing method for identifying the best low-dimensional descriptor in an immensity of offered candidates*. Phys. Rev. Mat. 2, 083802 (2018).

3) B. R. Goldsmith, M. Boley, J. Vreeken, M. Scheffler, and L. M. Ghiringhelli, *Uncovering structure-property relationships of materials by subgroup discovery.* New J. Phys. **19**, 013031 (2017).

4) A. Mazheika, Y. Wang, L. M. Ghiringhelli, F. Illas, S. V. Levchenko, M. Scheffler. *Ab initio data-analytics study of carbon-dioxide activation on oxide surfaces,* to be published.

COFFEE BEFORE THE COLLOQUIUM

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