UNIVERSITÄT DUISBURG ESSEN

PHYSIK E=

Physikalisches Kolloquium

Mittwoch, 24.04.2024
13:00 Uhr
MC 122 und Zoom

https://uni-due.zoom-x.de/j/64228670246?pwd=RjVQeFNIUkRKRkpiNVpKYXhJaFNLdz09

AI guided workflows for efficiently screening the materials space:
Examples for thermal insulators and heterogeneous catalysis

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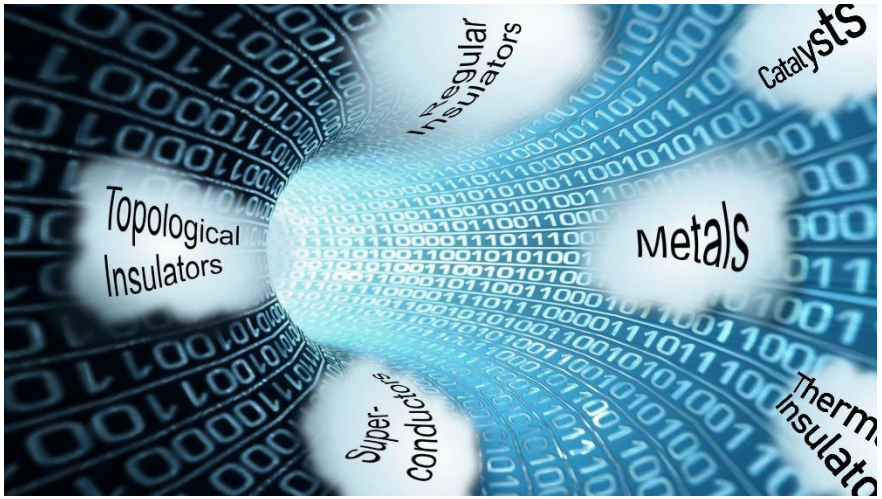

Artificial intelligence (AI) may capture the properties and functions of materials better than previous theoretical/computational methods because it targets correlations and does not assume a single, specific underlying physical model. Thus, it addresses the full intricacy of the numerous processes that govern the function of materials. However, the statistical analysis and interpretation of AI models require careful attention.

In this talk I will discuss recently developed, explainable AI methods [1,2] and applications [3-5] that combine detailed, consistent experimental data (called “clean data”) with theoretical data for the identification of “rules” that determine the properties and functions of materials. These “rules” depend on descriptive parameters, called “materials genes”. In analogy to genes in biology they are correlated with a certain material property or function. Thus, these materials genes help the identification of materials that are, for example, better electrical conductors or better heat insulators or better catalysts.

(*) Work done in collaboration with Lucas Foppa, Thomas Purcell, et al.

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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); https://doi.org/10.1103/PhysRevMaterials.2.083802
3. L. Foppa, L.M. Ghiringhelli, F. Girgsdies, M. Hashagen, P. Kube, M. Hävecker, S. Carey, A. Tarasov, P. Kraus, F. Rosowski, R. Schlögl, A. Trunschke, and M. Scheffler, *Materials genes of heterogeneous catalysis from clean experiments and artificial intelligence.* MRS Bulletin **46** (2021); https://doi.org/10.1557/s43577-021-00165-6
4. L. Foppa, C. Sutton, L. M. Ghiringhelli, S. De, P. Löser, S.A. Schunk, A. Schäfer, and M. Scheffler, *Learning design rules for selective oxidation catalysts from high-throughput experimentation and artificial intelligence.* ACS Catalysis **12**, 2223 (2022); https://doi.org/10.1021/acscatal.1c04793
5. T. Purcell, M. Scheffler, L. M. Ghiringhelli, C. Carbogno, *Accelerating Materials-Space Exploration by Mapping Materials Properties via Artificial Intelligence: The Case of the Lattice Thermal Conductivity.* npj Comput Mater **9**, 112 (2023); https://doi.org/10.1038/s41524-023-01063-y