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Einladung zum Vortrag

"Data-driven materials science: towards interpretable maps of materials properties"

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Ort: **Victor-Franz-Hess-Hörsaal, Währinger Straße 17,**
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Abstract:
The number of possible materials is practically infinite, while only few hundred thousands of (inorganic) materials are known to exist and for few of them even basic properties are systematically known. In order to speed up the identification and design of new and novel optimal materials for a desired property or process, strategies for quick and well-guided exploration of the materials space are highly needed. A desirable strategy would be to start from a large body of experimental or theoretical data, and by means of artificial-intelligence (AI) methods, to identify yet unseen patterns or structures in the data, and consequentially predictive (data-driven) models. This leads to the identification of maps (or charts) of materials where different regions correspond to materials with different properties. The main challenge on building such maps is to identify the appropriate descriptive parameters (called descriptors) that define these regions of interest.
Here, I present novel methods, based on sparse regression, for the AI-aided identification of descriptors and materials maps, tailored to work (also) with "small-data" and identify simple, in a sense human interpretable, models. The methods are applied to the prediction of topological insulators, of perovskites' stability, of CO2 activation on metal-oxide surfaces, and more.
I focus on the (verified) predictive power of the learned maps, which goes beyond the mere interpolation of more "popular" AI approaches, and analyze current and future

Im Rahmen des Vortrages findet eine Lehrprobe zum Thema „The quantum harmonic oscillator" statt.