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Nichtgleichgewichtsdynamik kondensierter Materie in der Zeitdomäne

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AI-Ready materials-science FAIR data: methods and infrastructure

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To accelerate the identification and design of optimal materials for a desired property or process, strategies for a well-guided exploration of the materials space are highly needed. A desirable strategy would be to start from a consistent body of experimental or theoretical data, and by means of artificial-intelligence (AI), to identify yet unseen patterns in the data, and consequentially predictive, data-driven models. This leads to the identification of materials' (properties) maps, where different regions correspond to materials with different properties. The main challenge on building such maps is to find the appropriate descriptive parameters (called descriptors) that define these regions of interest.

Here, I present recent updates on novel methods for the AI-aided identification of descriptors and materials maps, tailored to work (also) with "small-data", and applied to important materials-science challenges such as the prediction of mechanical properties of perovskite materials, of catalytic properties of experimentally characterized materials, and more.

Furthermore, I will introduce the NOMAD AI toolkit, an online platform for publishing and sharing curated Jupyter notebooks for the tutorial introduction of old and new AI tools and for providing an interactive access to AI workflows as published in peer-reviewed journals. In this way, new and experienced researchers can fully benefit of the community's advancements and reproducibility in science can meet its full potential.

Für diese Zeit steht eine Kinderbetreuung nach vorheriger Anmeldung zur Verfügung.

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