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TOPICAL REVIEW

AI guided workflows for efficiently screening the materials space

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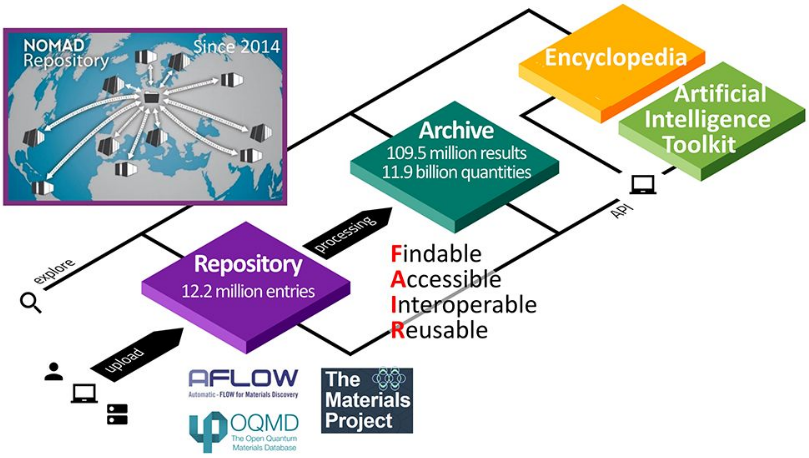
Author introduction

Matthias Scheffler is a theoretical physicist whose research focuses on condensed matter theory, materials science, and artificial intelligence. He is particularly known for his contributions to density-functional theory and many-electron quantum mechanics and for his development of multiscale approaches. In the latter, he combines electronic-structure theory with thermodynamics and statistical mechanics and employs numerical engineering methods. As summarized by his appeal "Get Real!", he introduced environmental factors (e.g. partial pressures, deposition rates, and temperature) into *ab initio* calculations. In recent years, he has increasingly focused on data-centric scientific concepts and methods (the fourth paradigm of materials science) and on the goal that materials-science data must become "Findable and Artificial Intelligence Ready."



AI guided workflows for efficiently screening the materials space

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Abstract 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. Therefore, 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.
The review article started with a brief discussion of historical aspects of data-centric science. It then focused on the recently developed, explainable AI methods [8,10] and applications [2,11,12]. The identified "rules" determine the properties and functions of materials. The rules depend on descriptive parameters called "materials genes." As genes in biology, they are correlated with a certain material property or function. Thus, these materials genes help to identify materials that are, for example, better electrical conductors or better heat insulators or better catalysts.

Keywords artificial intelligence, machine learning, active learning, symbolic regression, materials science, materials genes.

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