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Novel tools for accelerated materials discovery in the AFLOWLIB.ORG repository: breakthroughs and challenges in the mapping of the materials genome[1]

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High-Throughput Quantum-Mechanics computation of materials properties by ab initio methods has become the foundation of an effective approach to materials design, discovery and characterization. This data driven approach to materials science currently presents the most promising path to the development of advanced technological materials that could solve or mitigate important social and economic challenges of the 21st century. In particular, the rapid proliferation of computational data on materials properties presents the possibility to complement and extend materials property databases where the experimental data is lacking and difficult to obtain. Enhanced repositories such as AFLOWLIB, open novel opportunities for structure discovery and optimization, including uncovering of unsuspected compounds, metastable structures and correlations between various properties. The practical realization of these opportunities depends on the the design effcient algorithms for electronic structure simulations of realistic material systems, the systematic compilation and classification of the generated data, and its presentation in easily accessed form to the materials science community, the primary mission of the AFLOW consortium.

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