High-throughput computational screening

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The new field of high-throughput ab-initio materials modeling has been raising considerable interest in the last decade [1, 2]. This is due to the conjunction of two recent developments: the increasing availability of computational data, and the achievements obtained by machine-learning methods based on such large datasets. While the search for new materials with improved properties has been a long-standing issue, this new route is already showing its capacity to accelerate drastically the experimental discovery of new materials [3, 4, 5, 6].

High-throughput computing has been originally pushed forward by groups in the U.S., giving birth to large databases such as the Materials Project or AFLOWlib. Europe is now increasingly investing in this field, with groups at the state of the art in different countries and large European projects such as the NOMAD and AiiDA repositories. At present, several challenges remain to be solved. For example, to improve the prediction of the (meta-)stability of compounds, notably at finite temperature; to accelerate more advanced electronic structure methods so that they can be used high-throughput; or more practically, to tighten the links with experiments and industrial developments.

With this colloquium, we aim at bringing together the international community of high-throughput computational screening. For this reason, we welcome contributions in English.

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