High-throughput computational screening

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Keywords: High-throughput, ab-initio calculations, machine learning, materials science

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 com-
putational screening. For this reason, we welcome contributions in English.

References

(2013).


