

MAR15-2014-020333

Abstract for an Invited Paper
for the MAR15 Meeting of
the American Physical Society

Structuring intuition with theory: The high-throughput way¹

MARCO FORNARI, Department of Physics and Science of Advanced Materials Program, Central Michigan University

First principles methodologies have grown in accuracy and applicability to the point where large databases can be built, shared, and analyzed with the goal of predicting novel compositions, optimizing functional properties, and discovering unexpected relationships between the data. In order to be useful to a large community of users, data should be standardized, validated, and distributed. In addition, tools to easily manage large datasets should be made available to effectively lead to materials development. Within the AFLOW consortium we have developed a simple frame to expand, validate, and mine data repositories: the MTFrame. Our minimalistic approach complement AFLOW and other existing high-throughput infrastructures and aims to integrate data generation with data analysis. We present few examples from our work on materials for energy conversion. Our intent s to pinpoint the usefulness of high-throughput methodologies to guide the discovery process by quantitatively structuring the scientific intuition.

¹This work was supported by ONR-MURI under contract N00014-13-1-0635 and the Duke University Center for Materials Genomics