THEOS
THEORY AND SIMULATION OF MATERIALS

MARVEL
NATIONAL CENTRE OF COMPETENCE IN RESEARCH

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

Database driven computational materials discovery: the OQMD and its applications

Vinay I. Hegde,
The Wolverton Group, Department of Materials Science and Engineering, Northwestern University, IL 60208, USA

Tuesday August 23, 11:00, Room MED2 1522

Abstract: The advent of high-throughput databases populated with ab initio calculations of hundreds of thousands of compounds has given rise to new paradigms in computational materials discovery: based on (a) multistep-screening of various structural prototypes, (b) training models on large amounts of data using machine learning algorithms, and (c) significantly reducing the target space for sophisticated global structural search methods. One such high-throughput database is the Open Quantum Materials Database (OQMD) developed in the Wolverton group at Northwestern University. The talk will provide an overview of the OQMD, including available data, accessibility, and functionalities. Further, examples of its use in discovering new materials for various applications such as high-strength alloys, batteries, thermochemical water-splitting, and thermoelectrics will be discussed in the context of the three discovery paradigms mentioned above.