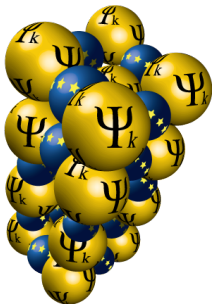
MARVEL

NATIONAL CENTRE OF COMPETENCE IN RESEARCH

MAX DRIVING THE EXASCALE TRANSITION



MARVEL/MaX/Psi-k Tutorial on high-throughput computations: general methods and applications using AiiDA

Highlight talk 1

Thomas Bligaard
Stanford University, USA

Accelerating high-throughput simulations using machine learning methods

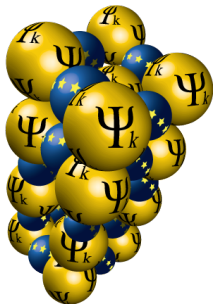
Modern machine learning techniques allows one to fit (non-linear) models with many unknown parameters while maintaining control of issues relating to overfitting. When moving towards massively high-throughput simulations many parts of the simulations can benefit from being integrated with machine learning. Examples relate to improved initial guesses, faster search algorithms using surrogate machine learning models, systematic error estimation, reduction of model complexity, and improved simulation model accuracy.

Highlight talk 2

Stefano Sanvito
Trinity College Dublin, IRL

High-throughput electronic structure theory: do we need to calculate always everything?

The development of novel materials is a strong enabler for any technology, and often technology and materials innovation cannot be separated. Unfortunately, the process of finding new materials, optimal for a given application, is lengthy, often unpredictable and has a low throughput. Here I will describe a systematic pathway to the discovery of novel materials, which demonstrates an unprecedented throughput and discovery speed. The method can be applied to any materials class and any potential application. I will use the example of magnetism to introduce the main features of the method, and I will demonstrate the discovery of several new high-performance magnets. Furthermore, I will highlight how such high-throughput schemes can be combined with machine-learning methods for data-mining to extract novel materials designing rules and for identifying new prototypes for further investigation.



Based on an extensive electronic structures library of Heusler alloys containing 236,115 prototypical compounds, we have filtered those alloys displaying magnetic order and established whether they can be fabricated at thermodynamical equilibrium. Specifically, we have carried out a full stability analysis for intermetallic Heuslers made only of transition metals. Among the possible 36,540 prototypes, 248 are found thermodynamically stable but only 20 are magnetic. The magnetic ordering temperature, TC, has then been estimated by a regression calibrated on the experimental TC of about 60 known compounds. As a final validation we have attempted the synthesis of a few of the predicted compounds and produced two new magnets. One, Co2MnTi, displays a remarkably high TC in perfect agreement with the predictions, while the other, Mn2PtPd, is a complex antiferromagnet. Our work paves the way for large-scale design of novel magnetic materials at unprecedented speed.

Highlight talk 3

Chris Pickard
University of Cambridge, UK

Random search as high throughput computation

The first principles computation of materials properties was once restricted to the investigation of a few structures at a time. The dramatic growth in the availability of computational resources now allows many thousands of computations to be performed independently and at the same time. One use of this power is to screen for novel or extreme materials, taking existing databases of crystal structures, or modifications of them, and computing their properties. While making use of existing knowledge of materials is an excellent starting point, in many cases, important structures are missing, not known, or even readily accessible. This is particularly the case for materials under extreme conditions, non-crystalline material structure, such defects – point defects, interfaces, or surfaces – and nano-structures.

To complement what we already know, it is essential to be able to make good, diverse and realistic, suggestions of possible structures at the atomic level. I will describe a straightforward approach to first principles structure prediction - Ab Initio Random Structure Searching (AIRSS) [1], and focus on the technical, high throughput, aspects of the method, from data acquisition to analysis and management.

[1] C. J. Pickard, and R. J. Needs, Journal of Physics-Condensed Matter, 23(5), 053201 (2011)

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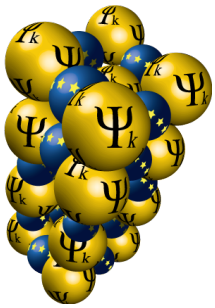

Highlight talk 4

Marco Fornari
Central Michigan University, USA

Structuring intuition with theory: The high-throughput

First principles methodologies have grown inaccuracy 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 successfully perform these tasks, however, specific property descriptors to link computable quantities with functionalities of interest must be defined. The story in this talk is organized around the concept of descriptors as a way to provide a structure for scientists' intuition and guide the discovery process.