Up-to-date approaches for atomistic material science.

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Machine learning (ML), a subfield of artificial intelligence, is currently used for various applications in materials sciences such as guiding chemical synthesis and discovery of new compounds, development of interatomic force fields and structural analysis of materials. This presentation proposes a review of ML techniques for an accurate description of the energy landscape and morphology of defects embedded into crystalline structure.

From atomic scale, multi-scale studies of properties in materials science face a traditional dichotomy in the choice of the atomistic force fields: robust, accurate and numerically expensive ab initio methods against less transferable but fast empirical methods [1]. The ML methods propose an intermediate approach that allows the control of the balance between the accuracy and numerical efficiency. Here, using the recently developed package MiLaDy (Machine Learning Dynamics) [2,3], we exemplify the case of energetic landscape of defects in metals. The present approach merges ab initio - free energy - machine learning regression (Kernel, Gaussian Processes, Polynomial) and, therefore, can provide quantities that underpin many multi-scale models, such as atomistic formation free energies or diffusion transition rates [4,5].

Moreover, the state-of-the-art ML methods combined with atomic descriptors are applied for automatic detection and structural analysis of defects in solids. Traditionally, structural analysis of defects is performed using well-established techniques, such as Wigner-Seitz, Voronoi and bond-angle analysis, etc. Here, we have opted for using semi-supervised ML techniques based at novelty/outlier detection, such as Support Vector Machine and Minimum Covariance Determinant. We firstly learn the bulk environment using deformations or standard molecular dynamics of bulk, without defects, supercells. Then, we perform the detection of the defects using the outlier detection techniques. Furthermore, based on this structural analysis technique, we also propose a generic numerical tool to examine transferability of kernel ML potentials, prior to perform time-consuming molecular dynamics calculations.

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