Machine Learning for Atomistic Materials Science

A.M. Goryaeva [1], T. D. Swinburne [2],
C. Lapointe [1], J. Baima [1], J. Dérès [1], M.-C. Marinica [1]

[1]*DEN - Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette, France*
[2]*CNRS, Centre Interdisciplinaire de Nanoscience de Marseille (CINaM), Université Aix-Marseille, France*

Multi-scale approaches 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. The ML methods propose a third avenue that allows control of the balance between the accuracy and numerical efficiency. Moreover, the ML-based vision of fundamental concepts in materials science, such as structural defects, can augment and revise traditional interpretations.
We will present recent advances in atomistic material simulations by means of machine learning and data-driven approaches.

Machine learning (ML) methods cannot fully replace traditional approaches in physics and/or materials science. The phase space in physics / materials science has a well defined structure and is too vast and complex to be described only by the inherent statistical correlations within the data points. Statistical methods trained on the physical data can be of great help when the traditional approaches are limited and/or their direct application is hindered by factors such as high computational cost.

In metals, the interaction and transformation of crystal defect networks give rise to an extraordinarily diverse range of defect morphologies [1]. Using the recently developed package MiLaDy (Machine Learning Dynamics) [2]: (i) we redefine the concept of defects in materials science [3]; (ii) we provide reliable force fields for complex defects such as interstitial, dislocation loops, dislocations; (iii) we are able to explore the atomistic free energy landscape of point defects in metals with *ab initio* accuracy up to the melting temperature [4], and, finally, (iv) we are able to propose surrogate models that bypass the traditional approaches [5]. We exemplify and discuss, in the framework of experimental findings, the case of energetic landscape of defects in body-centered and face-centered cubic metals.

[1] K. Arakawa , M.-C. Marinica *et al*. Nature Mater. **19**, 508 (2020) ; R. Alexander *et al*. Phys. Rev. B **94**, 024103 (2016)
[2] M.-C. Marinica, A. M. Goryaeva, T. D. Swinburne *et al*, MiLaDy - Machine Learning Dynamics, CEA Saclay, 2015-2021 ; A.M. Goryaeva, J.-B. Maillet, M.-C. Marinica. Comp. Mater. Sci. **166**, 200 (2019)
[3] A. M. Goryaeva *et al.* Nature Commun. **11**, 4691 (2020)
[4] C. Lapointe *et al.* (to be submitted); T.D. Swinburne, M.-C. Marinica, Phys. Rev. Lett. **120**, 135503 (2018)
[5] C. Lapointe, T. D. Swinburne *et al.* , Phys. Rev. Materials **4**, 063802 (2020); F. Bruneval *et al.* J. Chem. Theory Comput. **16**, 4399 (2020)