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Sampling Complex Energy Landscapes in Material Science Using Data-Driven Force Fields - Mihai Cosmin Marinica

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A. Zhong (1), C. Lapointe (1), A.M. Goryaeva (1), J. Wrobel (3), T. D. Swinburne (2), A. Allera (1), M. Athènes (1), M.-C. Marinica (1)

(1)DES - 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
(3) Faculty of Materials Science and Engineering, University of Technology, Wołoska 141, 02-507 Warsaw, Poland

Statistical methods, such as Machine Learning (ML) trained on physical data, can be invaluable when traditional approaches are limited or when their direct application is hampered by challenges like high computational costs. In materials science the interaction and transformation of crystal defects networks give rise to an extraordinarily diverse range of defect morphologies [1]. Additionally, accounting for chemical disorder presents another layer of complexity that is often overlooked in the emerging field of machine learning approaches. By utilizing the recently open-sourced MiLaDy (Machine Learning Dynamics) package [2] combined with accelerated Molecular Dynamics based on the Bayesian adaptive biasing force method [2], we aim to sample the intricate energy landscapes of defects by: (i) using methods that can identify complex networks of minima and saddle points at zero K; (ii) offering reliable force fields that handle intricate defects such as interstitials and dislocation loops; (iii) probing the atomistic free energy landscape of metals with ab initio accuracy up to the melting temperature [3]; (iv) examining chemical disorder in high entropy alloys (HEA); and, finally, (v) proposing surrogate models that sidestep traditional approaches to access challenging properties, like vibrational entropies [4].

[1] A. M. Goryaeva et al. Nature Commun. 14, 3003 (2023); A. M. Goryaeva et al. Nature Commun. 11, 4691 (2020);
[2] M.-C. Marinica, A. M. Goryaeva, T. D. Swinburne et al, MiLaDy - Machine Learning Dynamics, CEA Saclay, 2015-2023: https://ai-atoms.github.io/milady/ ;
[3] A. Zhong, C. Lapointe, A. M. Goryaeva, J. Baima, M. Athènes, and M.-C. Marinica„ Phys. Rev. Mater. 7, 023802 (2023); C. Lapointe et al. (to be submitted);
[4] C. Lapointe, et al. , Phys. Rev. Materials 4, 063802 (2020); C. Lapointe, et al, Phys. Rev. Materials 6, 113803 (2022).

Classification de Session: Challenge and Perspective