Charting nanocluster structures via convolutional neural networks

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A general method to obtain a representation of the structural landscape of nanoparticles in terms of a limited number of variables is proposed. The method is applied to a large data set of parallel tempering molecular dynamics simulations of gold clusters of 90 and 147 atoms, silver clusters of 147 atoms, and copper clusters of 147 atoms, covering a plethora structures and temperatures. The method leverages convolutional neural networks to learn the radial distribution functions of the nanoclusters and distills a low-dimensional chart of the structural landscape (figure 1). This strategy is found to give rise to a physically meaningful and differentiable mapping of the atom positions to a low-dimensional manifold in which the main structural motifs are clearly discriminated and meaningfully ordered. Furthermore, unsupervised clustering on the low-dimensional data proved effective at further splitting the motifs into structural subfamilies characterized by very fine and physically relevant differences such as the presence of specific punctual or planar defects or of atoms with particular coordination features [1]. The method has been successively enhanced in order to use the low dimensional description for the biasing of molecular simulations. In such a way, it made it possible to force and sample structural transitions in molecular dynamics simulations and to perform free energy calculations over the structural landscape of a system composed of 147 gold atoms (figure 2) [2].

References

[1] Telari, E., Tinti, A., Settem, M., Maragliano, L., Ferrando, R., & Giacomello, A. (2023). Charting nanocluster structures via convolutional neural networks. *ACS nano*, *17*(21), 21287-21296
[2] Telari, E., Tinti, A., Settem, M., Guardiani, C., Kunche, L. K., Rees, M., ... & Giacomello, A. (2025). Inherent structural descriptors via machine learning. *Reports on Progress in Physics*, *88*(6), 068002
[3] Authors, Journal, Issue (Year) page (Arial 10) Indicate references with sequential numbers within [square brackets].

Figures

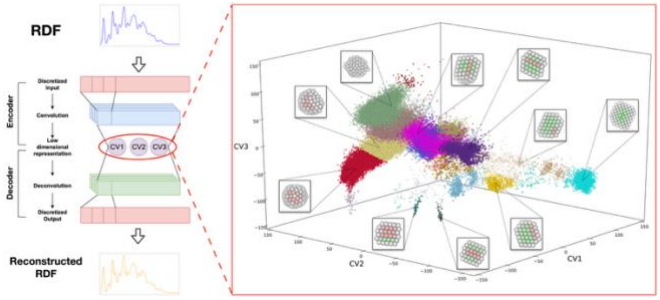

Figure 1. Sketch of the working principle of the convolutional neural network used to create the low dimensional space with an high-quality structural description of the system.

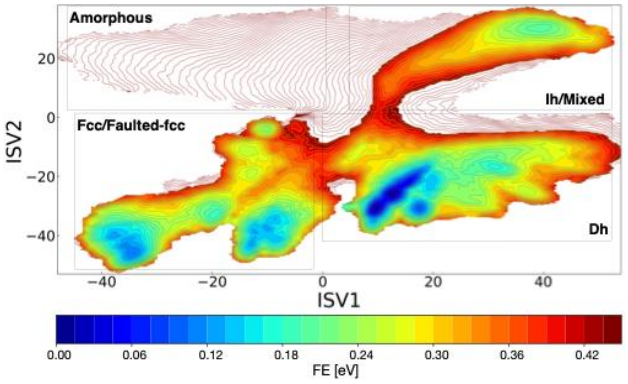

Figure 2. Free energy computed thanks to the low dimensional representation obtained via the autoencoder for Au_{147}.