The Φ-LassoLars method to construct Machine-learning interaction potentials

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Machine-learning methods have been recently employed to bridge the gap between classical interaction potentials and ab initio calculations by providing a framework to reach the accuracy of the latter while maintaining a low computational cost. In practice, Gaussian approximation potentials and Artificial Neural Network are the most popular techniques because they have shown promising results for lots of different systems including metals, oxides and carbonaceous materials.

As an alternative, in Φ-LassoLars, we propose the use of *(1)* a physically motivated expression for the potential and *(2)* a constrained linear regression scheme that allows to reduce the complexity of the obtained potential. In this talk, I will present in greater details the employed methodology and the results obtained on different materials.

**Bio: Julien Lam recently obtained a CNRS permanent position to work in CEMES (Toulouse). Prior to that, he did his postdocs in Brussels and Bristol as well as a PhD in Lyon. His research focuses on the study of crystallization mechanisms related to the formation of nanoparticles.*