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# Interatomic potentials from first principles

Abstract:

There is a new renaissance of interatomic potentials, they are now interpreted as surrogate models of the quantum mechanical potential energy surfaces. I will show how to define suitable representations of atomic coordinates and use regularised regression techniques, popular in machine learning nowadays, to achieve unprecedented accuracy in modelling hard and soft materials across a range of phases, including a wide variety of defects, allowing the study of phenomena previously unreachable using first principles approaches.