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ESI Erwin Schrödinger International Institute for Mathematics and Physics

Machine Learning for Materials Hard and Soft

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Introduction to Electronic Structure Methods

Abstract:
We present an overview of some of the widely used electronic structure methods, including density functional theory, Hartree-Fock, coupled cluster and quantum Monte Carlo, and connect these approaches with recent advances using machine learning. We will focus on the key concepts and techniques for one such method, variational Monte Carlo, where deep learning has had a considerable impact in the last few years.

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