Implementation of a Machine Learning Force Fields Platform for Quantum Dots

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Quantum dots (QDs) are nanoscale semiconductor particles that exhibit size- and shape-dependent electronic and optical properties, making them highly versatile for applications in optoelectronics, photovoltaics, and biomedical imaging. However, simulating their dynamic behavior and intricate electronic structure -particularly in molecular dynamics (MD)- remains a challenge. Traditional force fields often lack the specificity to account for the unique structural and electronic environments within QDs, while *ab initio* methods -though accurate- are prohibitively expensive for large-scale or long-timescale simulations. This gap motivates the development of more efficient yet accurate approaches to model QD systems.

Here, we introduce a novel automated platform for developing machine learning (ML) force fields tailored to QDs. Leveraging the QMflows software [1], our framework integrates high-level quantum mechanical data with advanced ML training frameworks available in the literature such as SchNetPack [2,3], DeepMD [4,5] and Allegro [6] (cf. Figure 1). This enables GPU-accelerated training of QDs for improved performance. By automating data collection, model training on various packages, and validation, the platform allows users to perform on-the-fly simulations with minimal parameter tuning. Recognizing that the accuracy and transferability of ML force fields depend strongly on the quality of the training data, we also provide smart data selection tools that prioritize sampling diverse and less-correlated structures from DFT calculations. This approach creates more informative training sets without requiring extensive data or incurring high computational costs.

A key strength of the platform is its ability to improve simulation accuracy without introducing additional computational overhead, achieving near *ab initio* accuracy at a cost closer to that of classical force fields. The platform's integration with QMflows makes it straightforward to create flexible workflows and link the resulting ML force fields to multiple quantum chemistry packages, with particular emphasis on the CP2K package [7].

Ultimately, this automated and computationally efficient framework contributes to the unification of quantum chemistry, machine learning, and materials science for the study and design of next-generation quantum dots.

References

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Figures

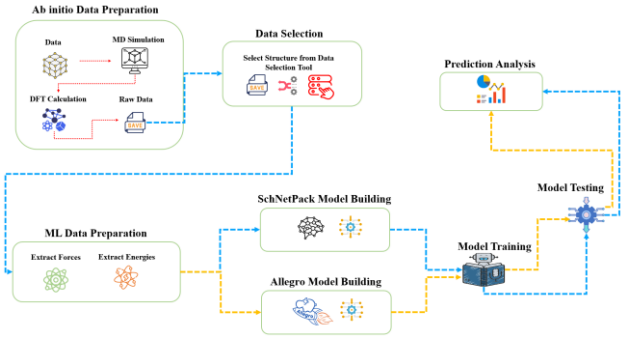

Figure 1. Arquitecture of the platform as implemented in QMFlows.