Efficient and Scalable Scheme for Predicting Potential Energies of Complex Material Systems with Quantum Neural Networks

HSU-KAI CHENG [1*], PO-YU YANG [1], CHUN-WEI PAO [1]

[1]Research Center for Applied Sciences, Academia Sinica, Taiwan

*E-mail: kaicheng0108@gmail.com

Introduction

- In our study, we propose a framework of leveraging quantum machine learning to predict the potential energy of a material system.
- We utilize two quantum machine learning models: quantum convolutional neural network (QCNN) and quantum deep neural network (QDNN).
- We adopt three types of descriptors, also known as atomic fingerprints, to represent our material systems: Atom centered symmetry functions (ACSF), Bispectrum of the neighbor density and Smooth overlap of atomic positions (SOAP).
- We employ two binning approaches to preprocess the descriptors prior data encoding.
- Our results show that by harnessing the binning approaches, it is possible to train a data- and parameter-efficient model that yields high prediction accuracy for complex material systems (up to five types of elements) of **arbitrary system sizes**.

Methodology

The flowchart of quantum machine learning framework is depicted in Fig.1, involving four steps: (1) feature generation (2) feature mapping/preprocessing (3) data embedding (4) model training.

(1) We first transform the atomic Cartesian coordinates onto a set of descriptors that would describe all equivalent representations of the system.

(2) Depending on the system size, the choice and the number of descriptors per atom directly impact the dimensionality of the space to be mapped. To address the issue of multi- and variable dimensions, two binning approaches are employed: (i) descriptors are sorted and renormalized according to the ranges of numerical values, as shown in Fig.1B (ii) descriptors are sorted and summed over the same type of atoms, as shown in Fig.1C

(3) Processed feature maps are then encoded into the corresponding qubit bases by performing amplitude embedding, as shown in Fig.1D.

(4) For our supervised learning task, we variationally optimize parameterized quantum circuits (QCNN and QDNN) over training data sets, and predict energies subsequently.

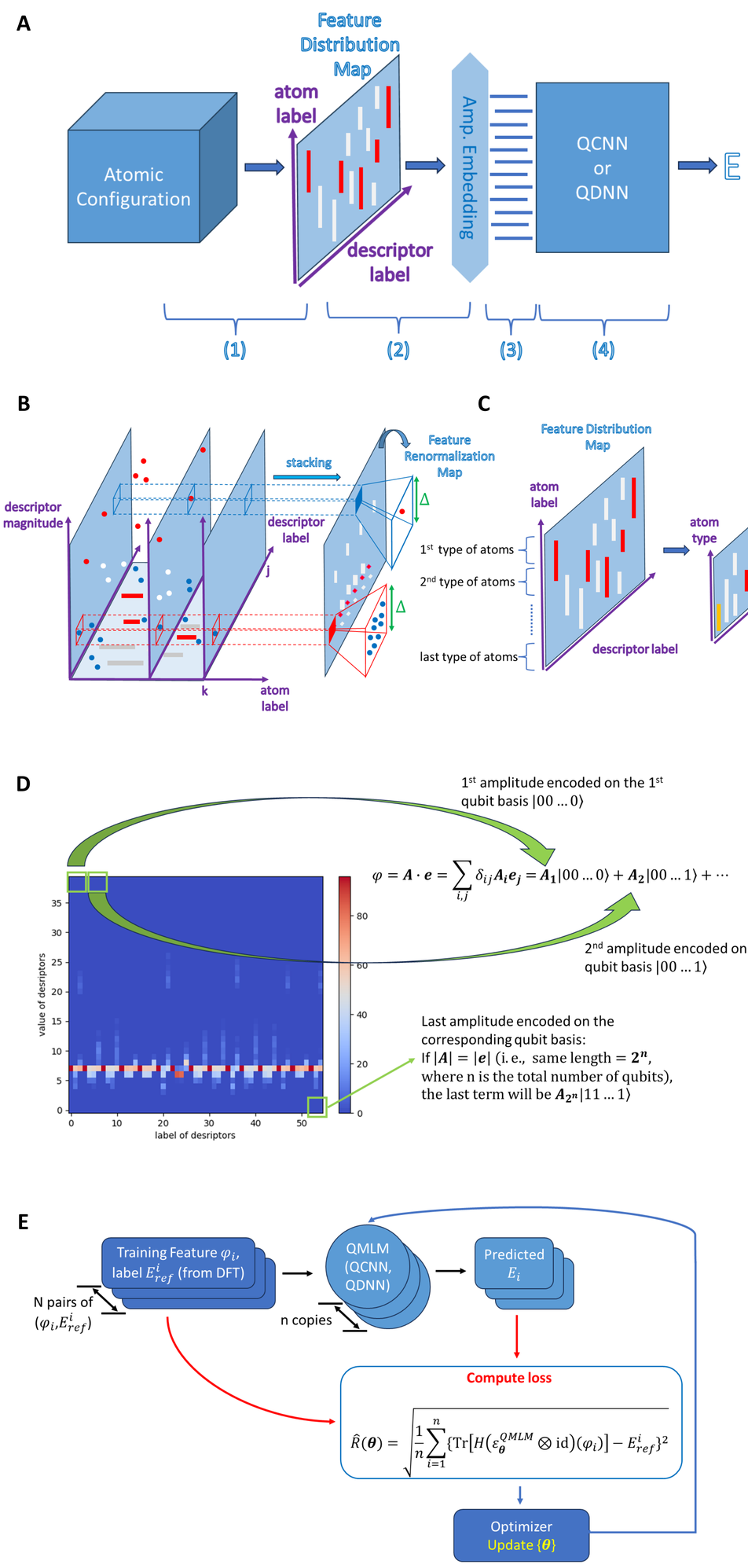


Fig.1 (A) The overall work flow of our quantum machine learning framework. (B) and (C) illustrates two binning approaches as shown in (A) step (2). (D) demonstrates the implementation of amplitude encoding as shown in (A) step (3) (E) portrays the training process: parameters within quantum machine learning models (QCNN and QDNN) are optimized and parallel computing is performed.

Quantum Machine Learning Model

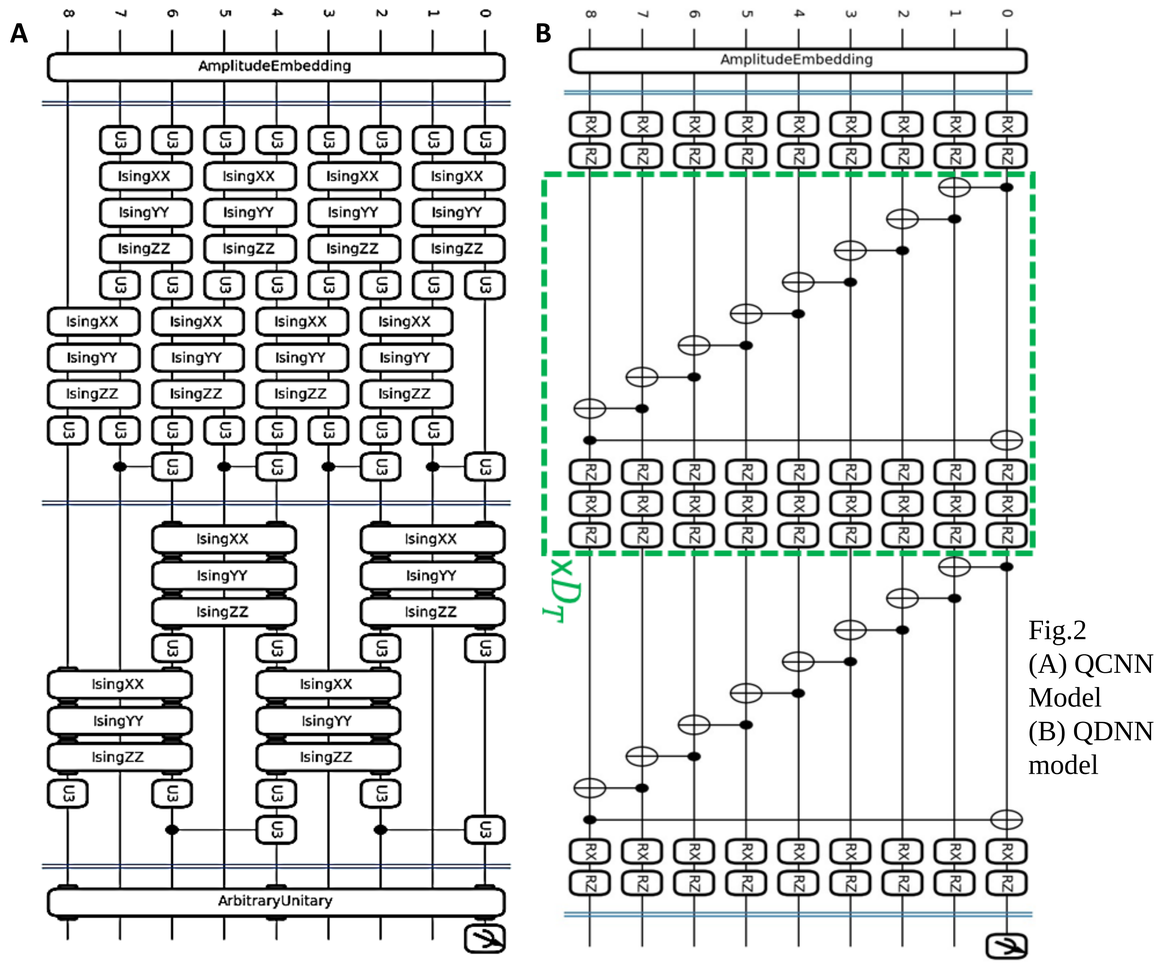
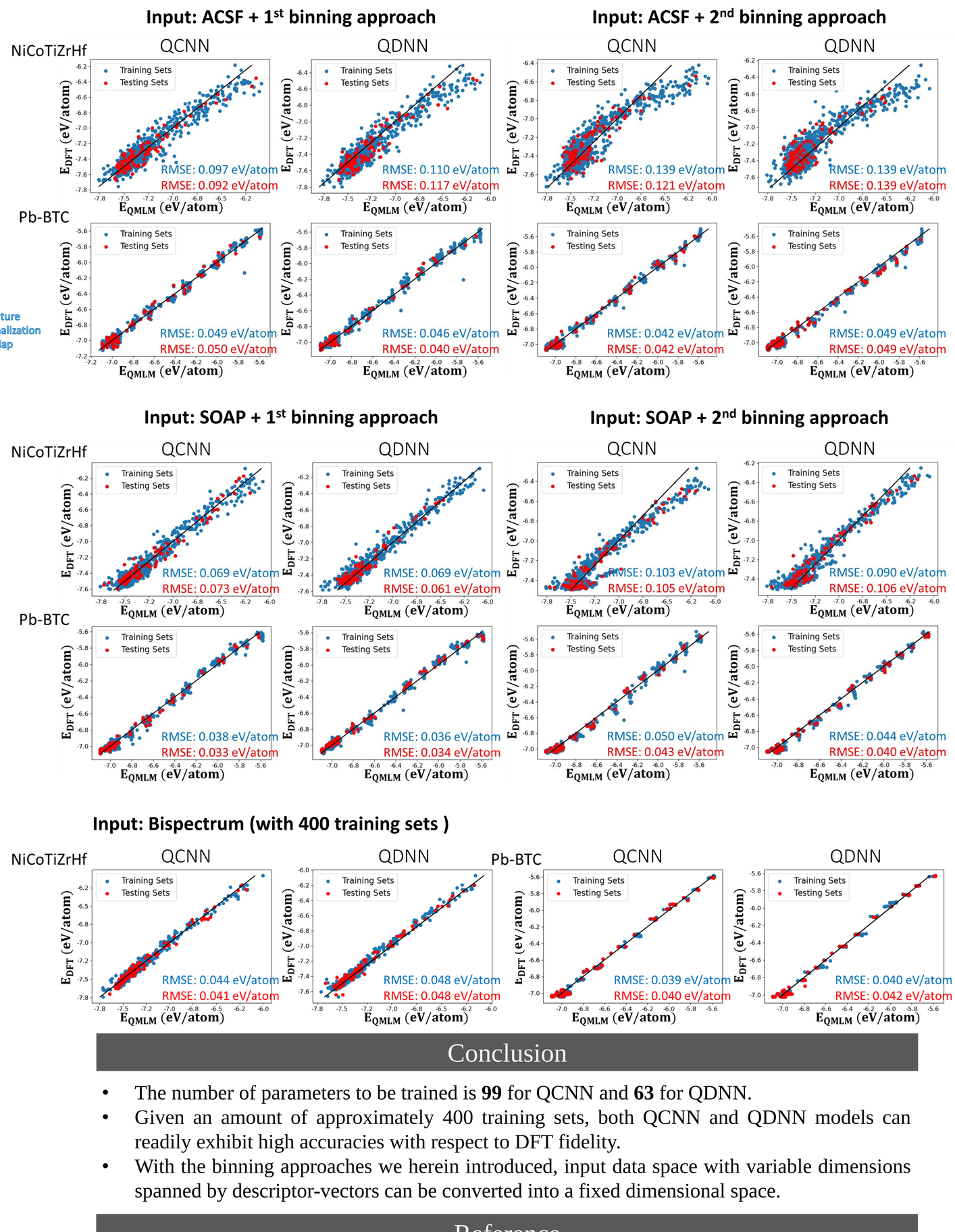


Fig.2
(A) QCNN Model
(B) QDNN model

Result

Two complex material systems are tested: (1) $Co_{25}Ni_{25}(HfTiZr)_{50}$, and (2) lead-based Metal–organic frameworks (MOFs) Pb-1,3,5-benzenetricarboxylate (Pb-BTC) with Li intercalation. Training/validation data are generated by density functional theory (DFT).

Energy Parity



Conclusion

- The number of parameters to be trained is **99** for QCNN and **63** for QDNN.
- Given an amount of approximately 400 training sets, both QCNN and QDNN models can readily exhibit high accuracies with respect to DFT fidelity.
- With the binning approaches we herein introduced, input data space with variable dimensions spanned by descriptor-vectors can be converted into a fixed dimensional space.

Reference

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