Quantum Neural Networks force fields generation

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Keypoint: We propose a quantum neural network (QNN) for the computation of energy and forces and use it successfully on simple molecules.

Paper: Kiss, *et al., Mach. Learn.: Sci. Technol.* **3** 035004 (2022)

Molecular Force Fields

1. **Goal:** compute the energy and forces between atoms in a molecule, given its configuration.

2. **Why:** Being able to run molecular dynamics (MD) by integrating Newton's equations of motion.

3. **Useful in:** computational physics, chemistry, material sciences, drug design, etc.

Methods:

1. **Approximate methods from first principles** (density-functional theory (DFT) or coupled clusters (CC):

   - precise

   - expensive and slow (on the fly) .

2. **Machine learning** (ML)

   - trained on DFT or experimental data set

   - really fast once trained

3. **Quantum neural networks:**

   - seems to be more expressive

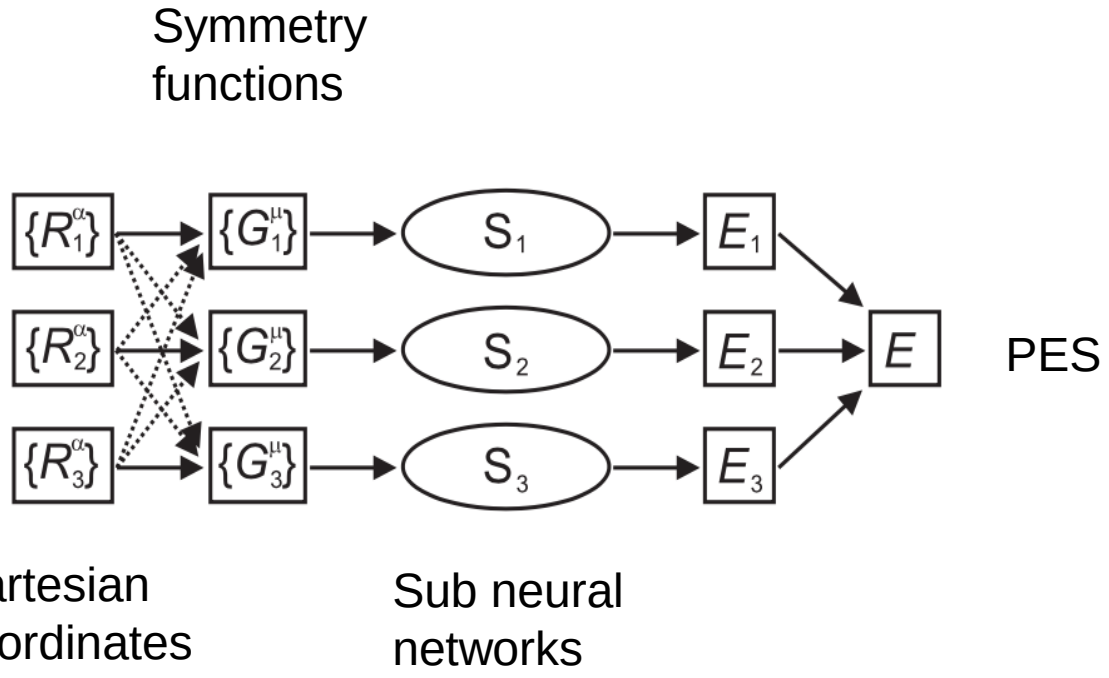
Classical NNs for Potential Energy Surface (PES) [1]

1. The model should respect the inherent **symmetry** of the system (***rotation, translation, permutation*** of the atoms of the same kind).

2. For every atom, a set of **symmetry functions** G_i^{μ} is constructed from the cartesian coordinates.

3. **Forces** are obtained as negative gradient of the PES:

$$F_{i,j} = -\frac{\partial E}{\partial R_i^j}$$



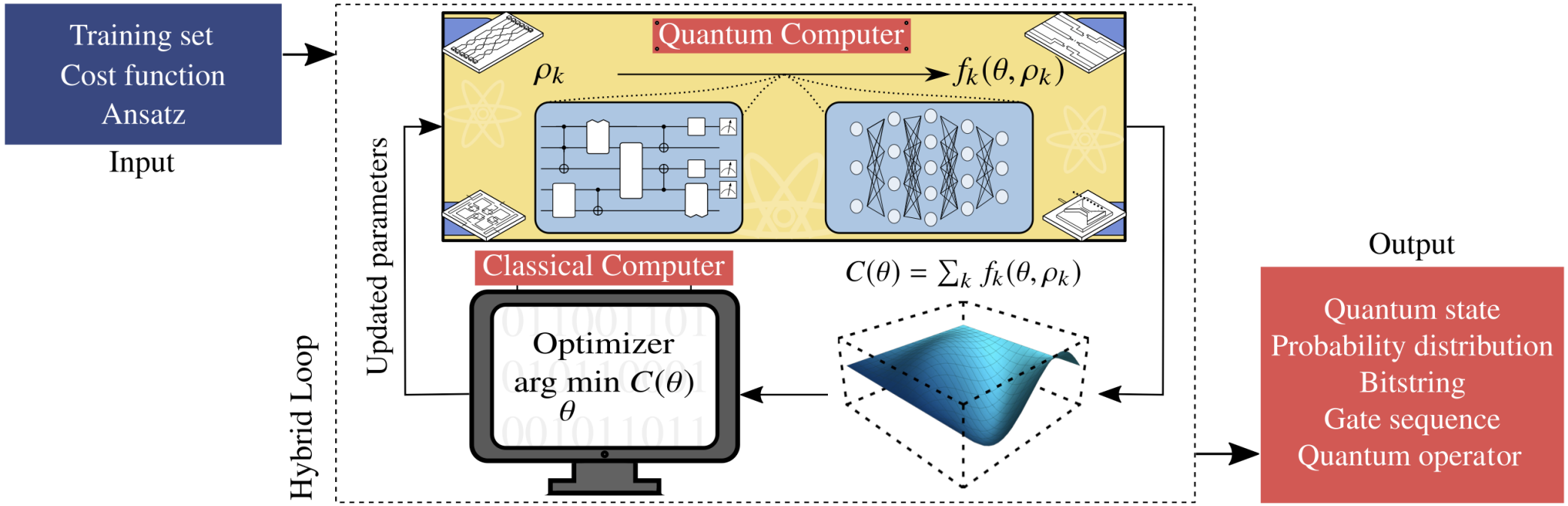
$$\mathcal{L}(x,\Theta) = \frac{1}{N}\sum_{n=1}^{N}(E^{(n)} - E_{exact}^{(n)})^2 + \frac{\chi}{3Na}\sum_{n,i,j}(F_{i,j}^{(n)} - F_{exact,i,j}^{(n)})^2$$

The **loss function** depends in general on both energy and forces.

[1] Jörg Behler and Michele Parrinello. *Generalized Neural-Network Representation of High-Dimensional Potential-Energy Surfaces*. In: Physical Review Letter 98, 146401 (Sept. 2006)

Quantum machine learning models

Quantum circuits as heuristic machine learning models.



Cerezo *et al.*, *Nat Rev Phys* **3**, 625–644 (2021)

Quantum Neural Networks

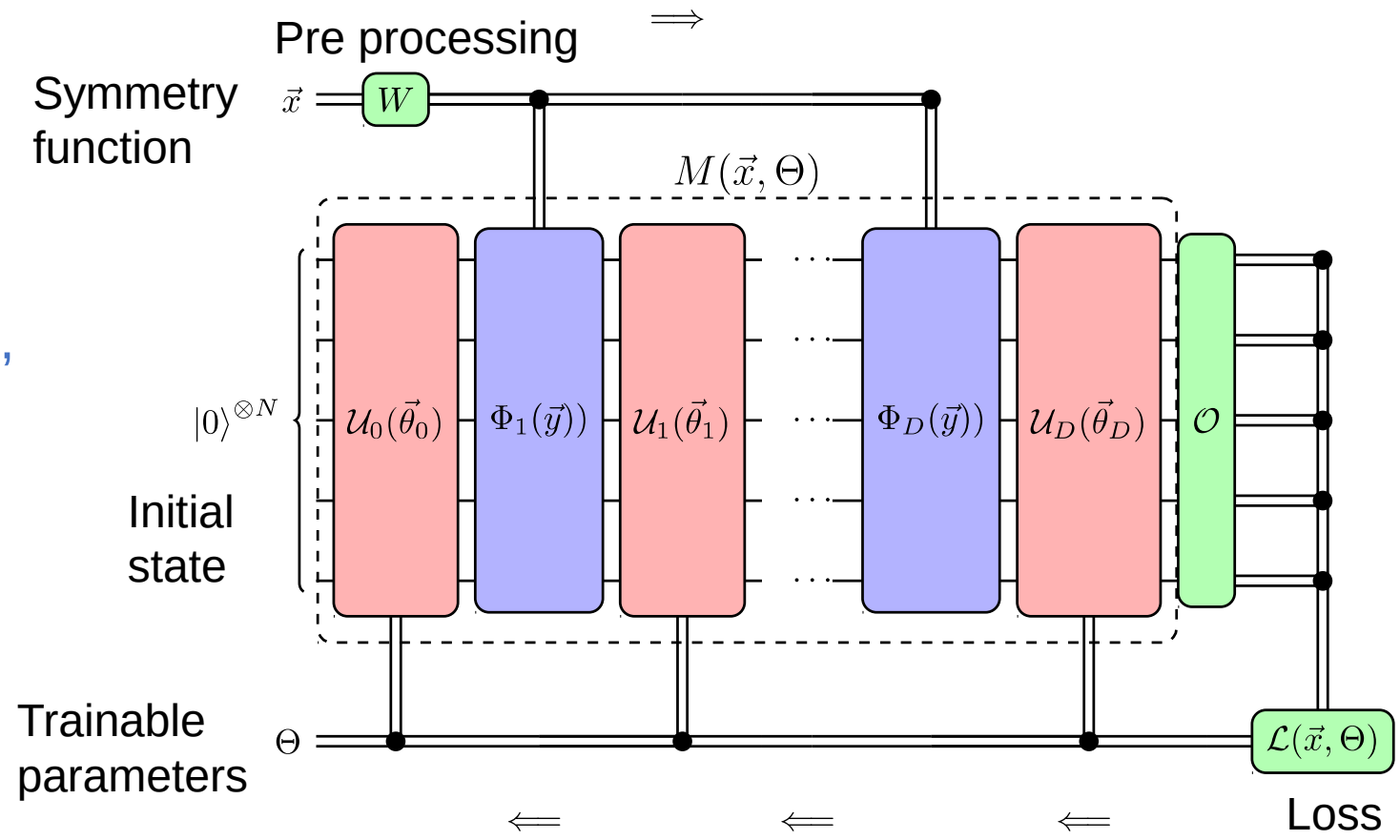
1. QNN: $f_\Theta(x) = \langle 0 | M^\dagger(x,\Theta)\mathcal{O}M(x,\Theta)|0\rangle$, M is the quantum circuit, $\mathcal{O} = \sigma_z^1$.

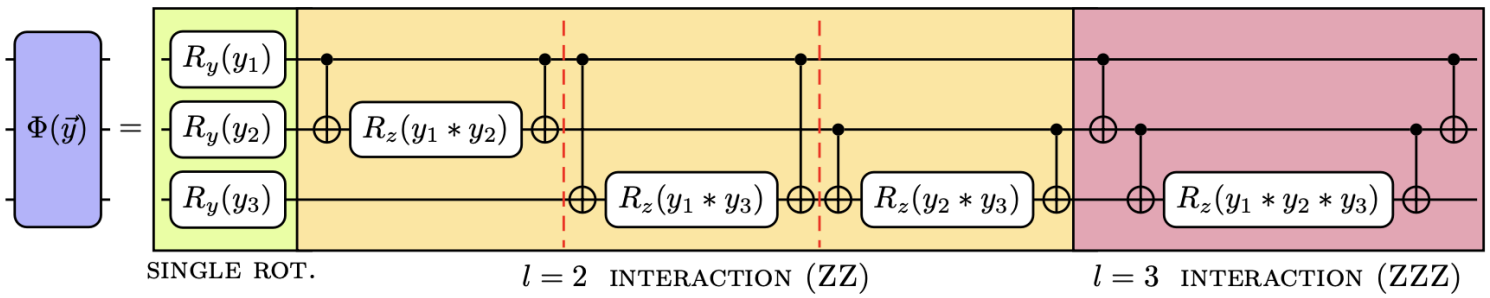
2. Partial Fourier series

   Schuld, *et al.*, *Phys. Rev. A* **103**, 032430 (2021)

3. Trainable: Hardware efficient ansatz.

4. Input: classical feature map W + repeated quantum feature map encoding to increase expressivity.





Kiss, *et al.*, *Mach. Learn.: Sci. Technol.* **3** 035004 (2022)

Application to Force Fields (Chemistry)

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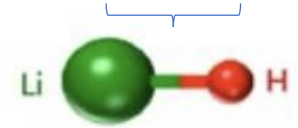
bond length r

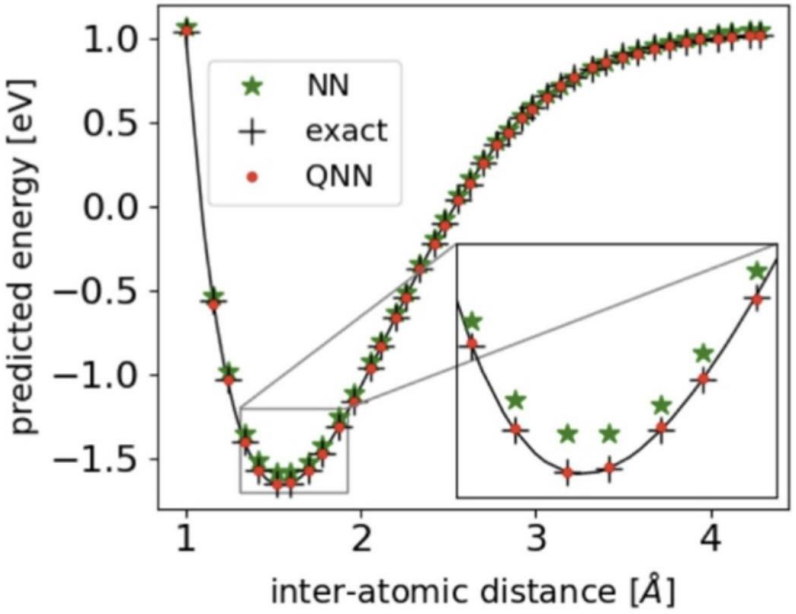
Li-H



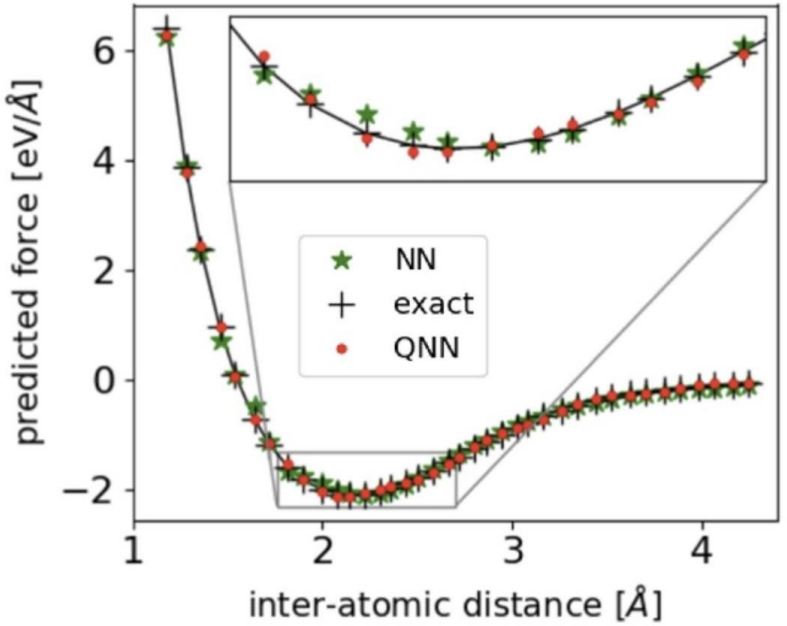
$$W : [-1,1] \to [-\pi,\pi]^3$$

$$r \mapsto \begin{pmatrix} \pi r \\ \arcsin(r) \\ \arccos(r) \end{pmatrix}$$

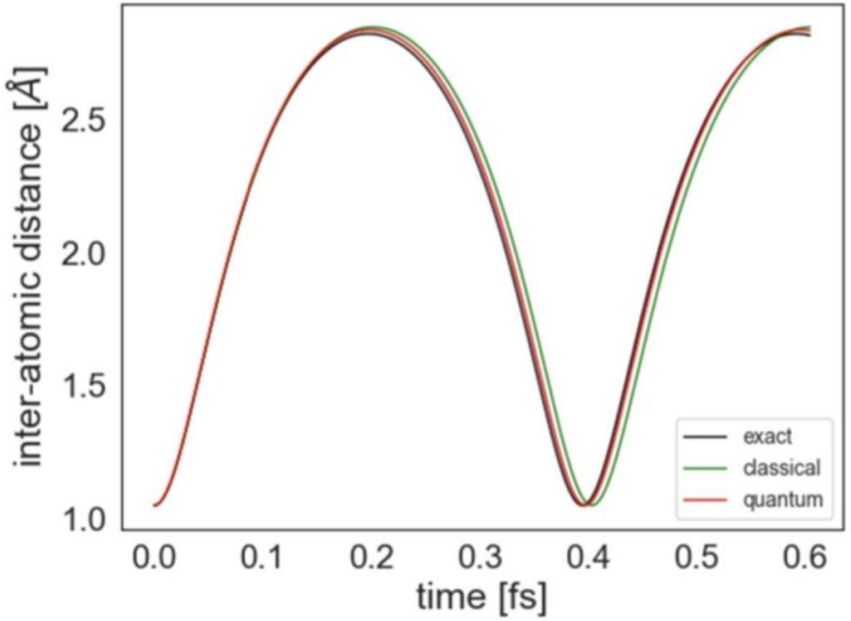
QNN with 10 layers (50 parameters)



(a) LiH Energy



(b) LiH Force



(a) Time evolution of the inter-atomic distance

Comparison with a neural network of equal complexity

$\vec{F} = -\vec{\nabla}_r E(r)$

Molecular Dynamics

Triatomic Molecule (H2O)

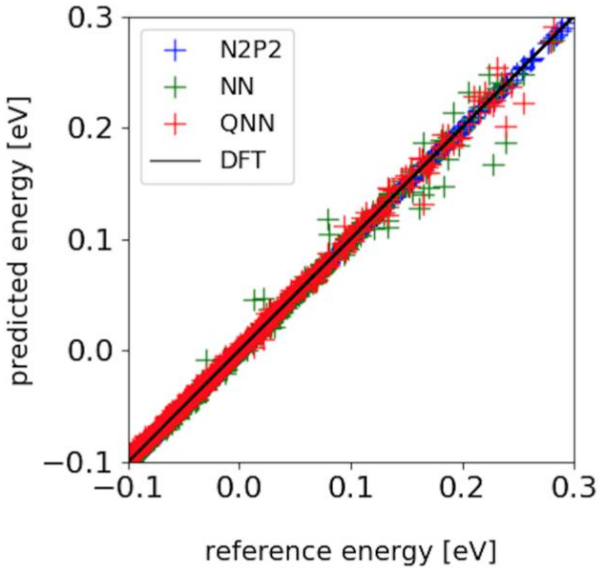
1. **3 degrees of freedom**: 1 angle, 2 bond lengths.
2. **Data Preprocessing**: scale between -1 and 1, apply W(x) = arcsin(x).
3. **Circuit design**: N=3, D=12, full feature map (l=3), full trainable feature map (l=3).
4. **Optimization:** Cobyla ($\chi = 1$) on 300 data points.

Effective dimension

H_2O	RMSE(E)	RMSE(F)	d_{300}/d	d
QNN	0.005	0.06	0.72	87
NN	0.006	0.1	0.25	87
n2p2	7×10^{-4}	0.01	0.04	1642

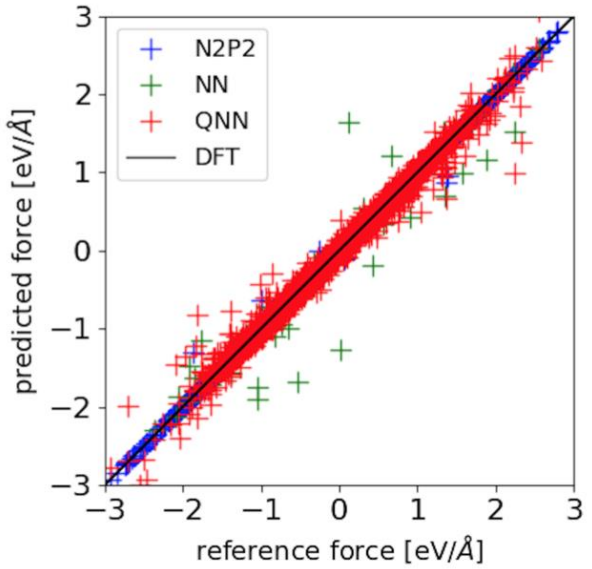
params

Energy



(a) H_2O Energy

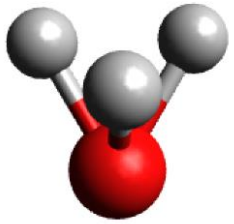
Forces



(b) H_2O Forces

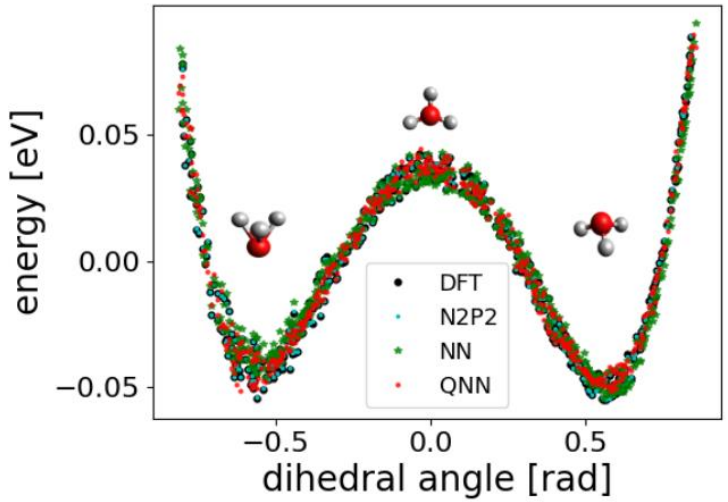
Abbas et al, *the power of quantum neural networks*, In Nat. Comput. Sci Comput. Sci **1** 403–409, (2021)

Umbrella motion of Hydronium (H_3O)

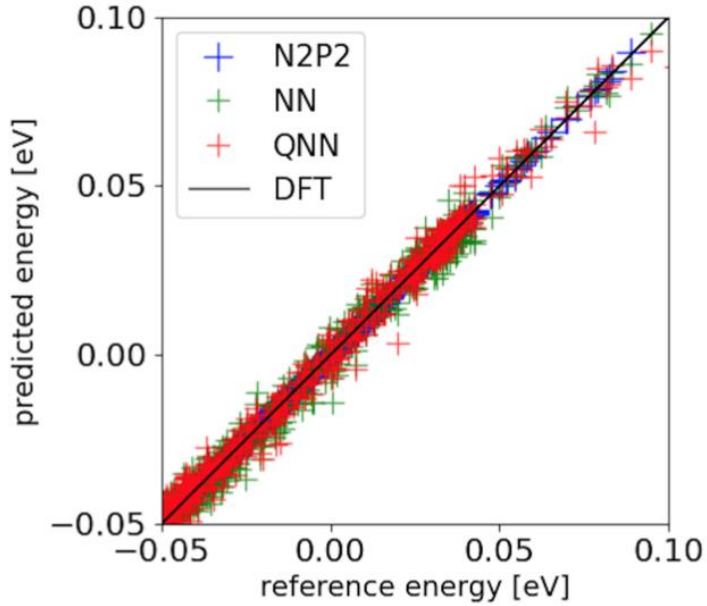


1. **6 degrees of freedom**: 1 dihedral angle, 2 angle, 3 bond lengths.
2. **Data Preprocessing**: scale between -1 and 1, apply W(x) = arcsin(x).
3. **Circuit design**: N=6, D=10, linear feature map (l=3), linear trainable feature map (l=3).
4. **Optimization:** ADAM ($\chi = 0$) on 500 data points.

H_3O^+	RMSE(E)	RMSE(F)	d_{500}/d	d
QNN	3.7×10^{-3}	0.26	0.67	135
NN	4.2×10^{-3}	0.207	0.19	135
N2P2	5×10^{-4}	0.19	0.03	2214



(a) H_3O Energy



(b) H_3O Energy

Conclusions, potential advantages & outlook

1. QNNs are able to compete with **similar neural networks** in the task of learning PES and force fields.

2. Potential quantum advantages are primarily linked to **the better expressivity and higher effective dimension** of QNNs with respect to classical counterparts.

3. **Future work**:

   - More complex architectures (**quantum convolutional NN**) or **equivariant QNN.**

   - Work with **quantum data** (from dynamical VQA).

   - Incorporate fragmentation techniques.

Thank you for your attention!
Questions?

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Schuld *et al.*, *Phys. Rev. A* **103**, 032430 (2021)
Abbas *et al.*, In Nat. Comput. Sci **1** 403–409, (2021)

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