Machine Learning the protonated water hexamer from Quantum Monte Carlo

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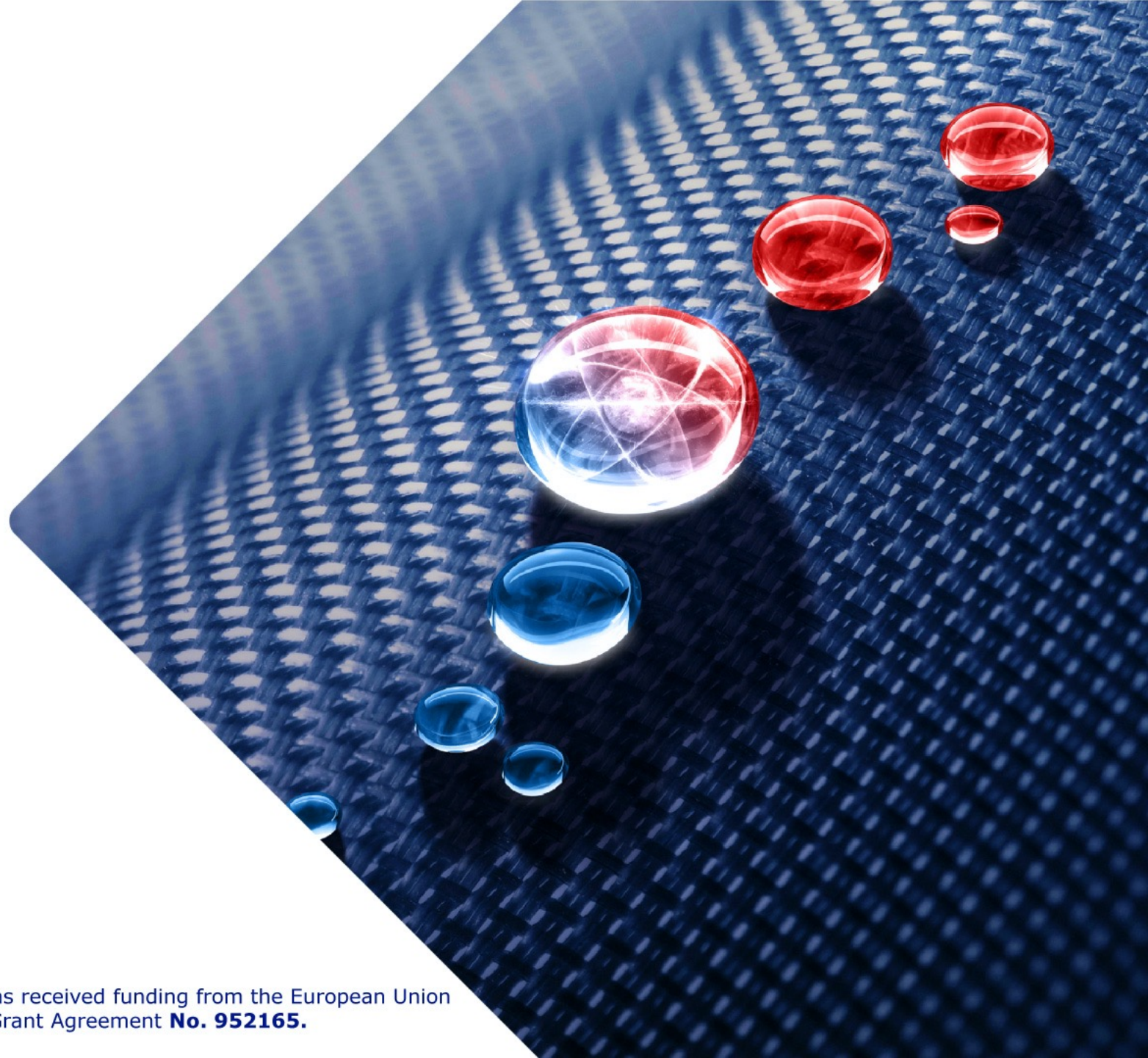

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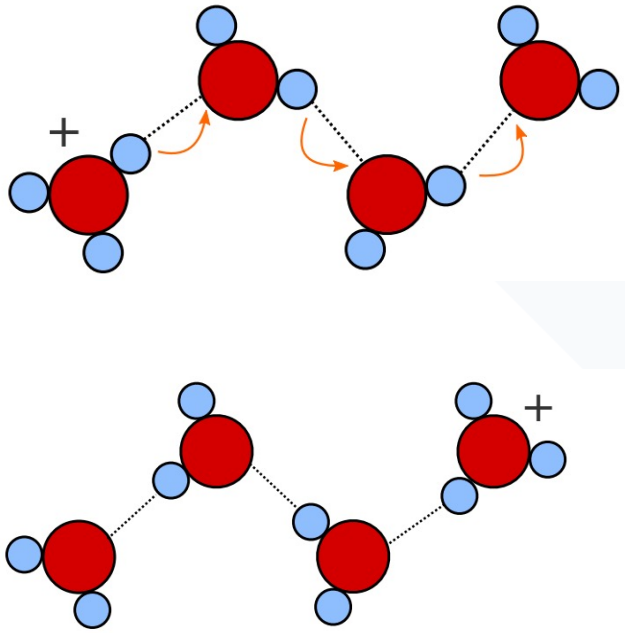
Outline

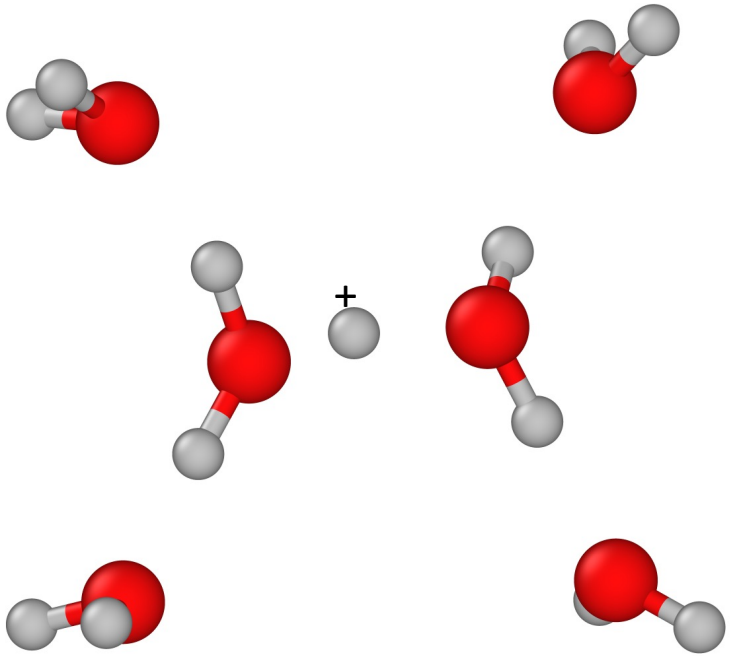
- Protonated water hexamer
- DFT vs QMC
- Machine Learning
- DFT vs ML(DFT)
- QMC vs ML(QMC)
- Perspectives

Proton transfer in the protonated water hexamer

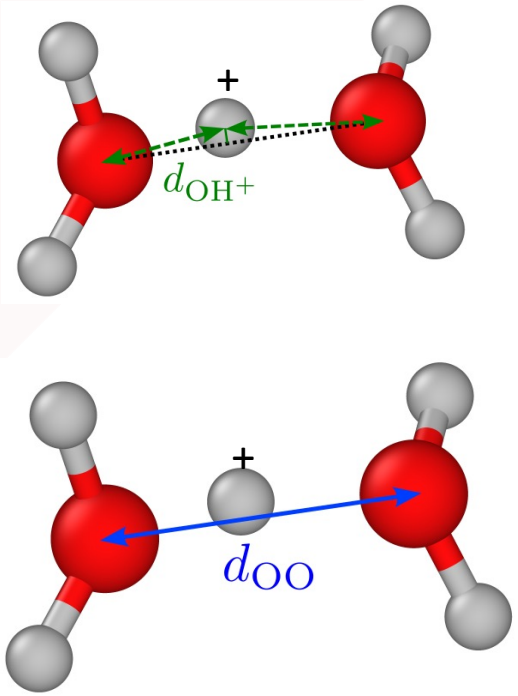
Grotthuss mechanism



Protonated water hexamer

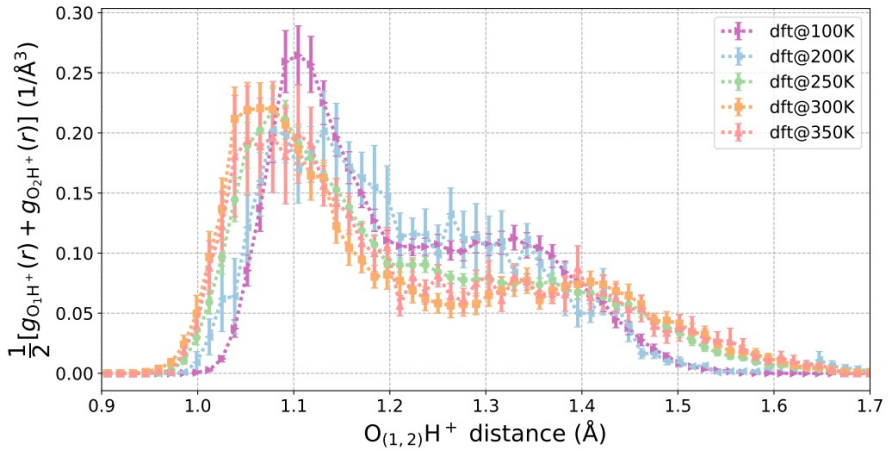


Coordinates

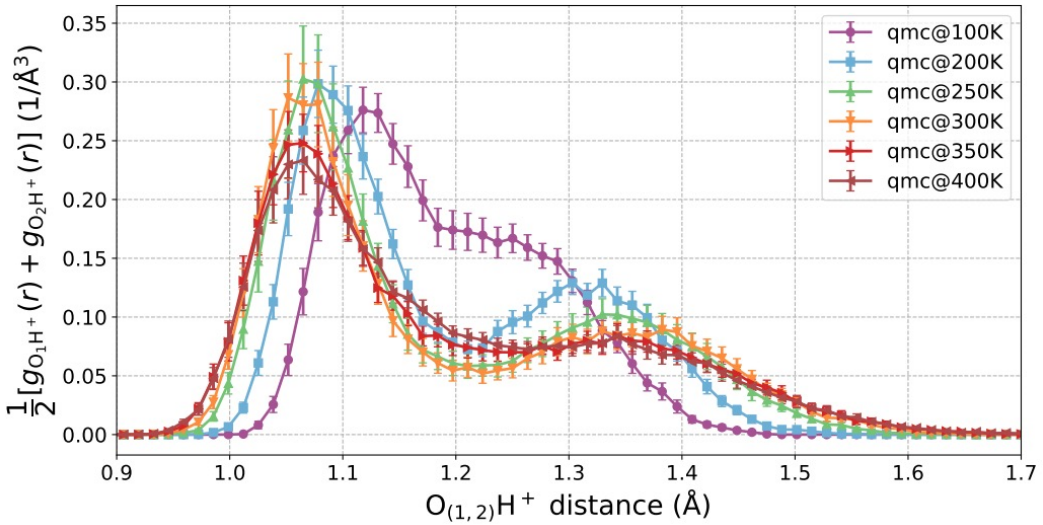


RDF DFT vs QMC

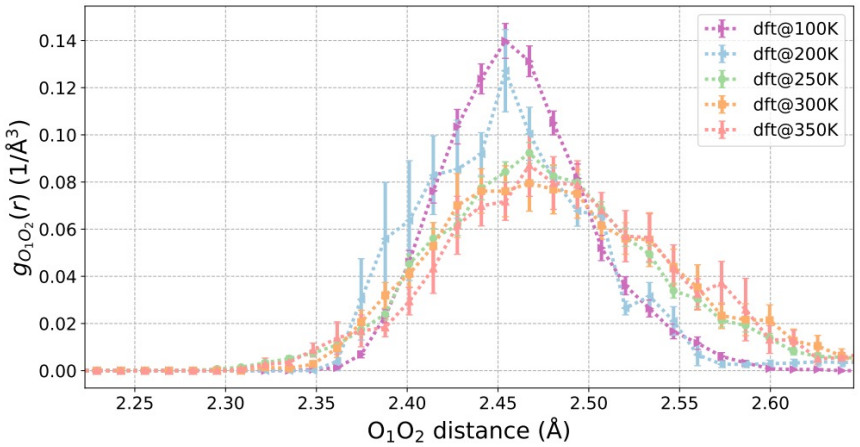
Symmetrized RDF $O_{(1,2)}$-H^+ from classic MD + **DFT** at different T



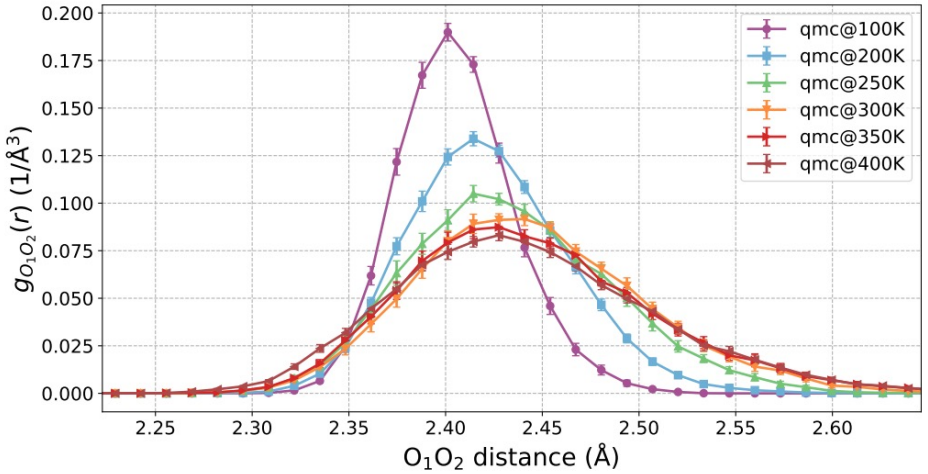
Symmetrized RDF $O_{(1,2)}$-H^+ from classic MD + **QMC** at different T



RDF O_1-O_2 from classic MD + **DFT** at different T

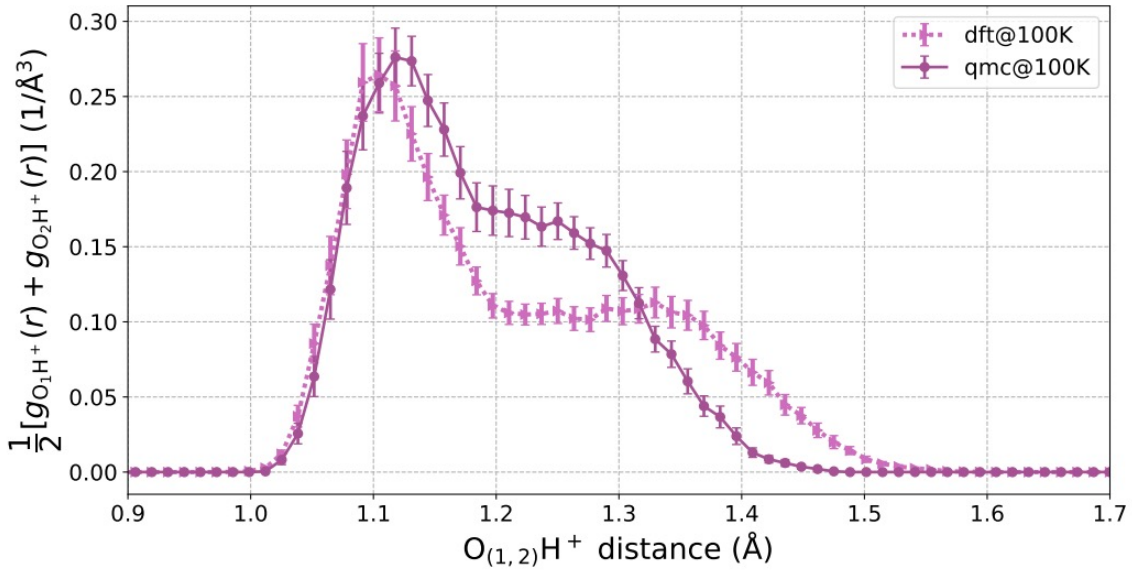


RDF O_1-O_2 from classic MD + **QMC** at different T

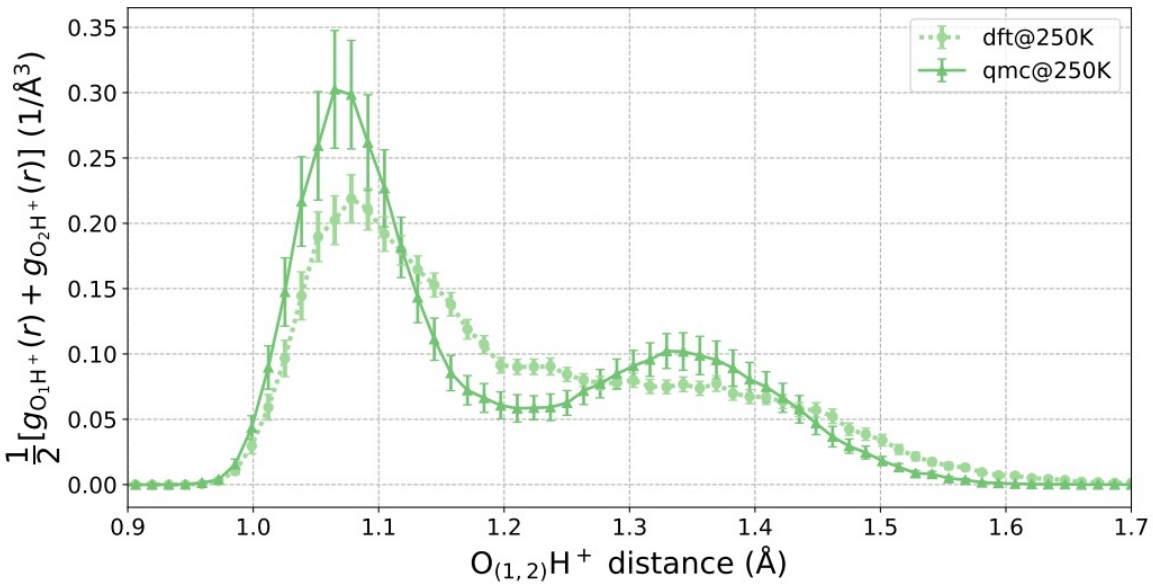


RDF DFT vs QMC (OH+ RDF differences)

Symmetrized RDF $O_{(1,2)}$-H^+ from classic MD at **100K** (QMC vs DFT)

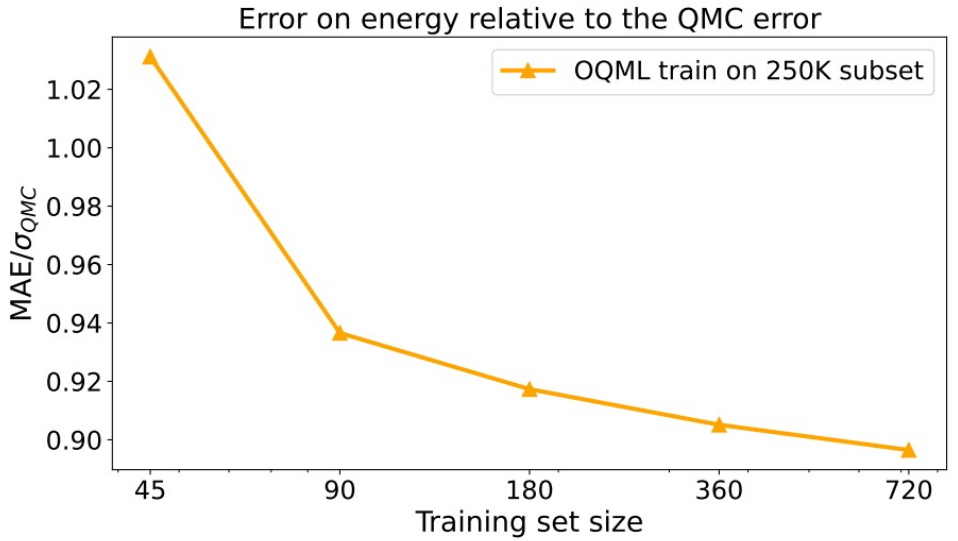


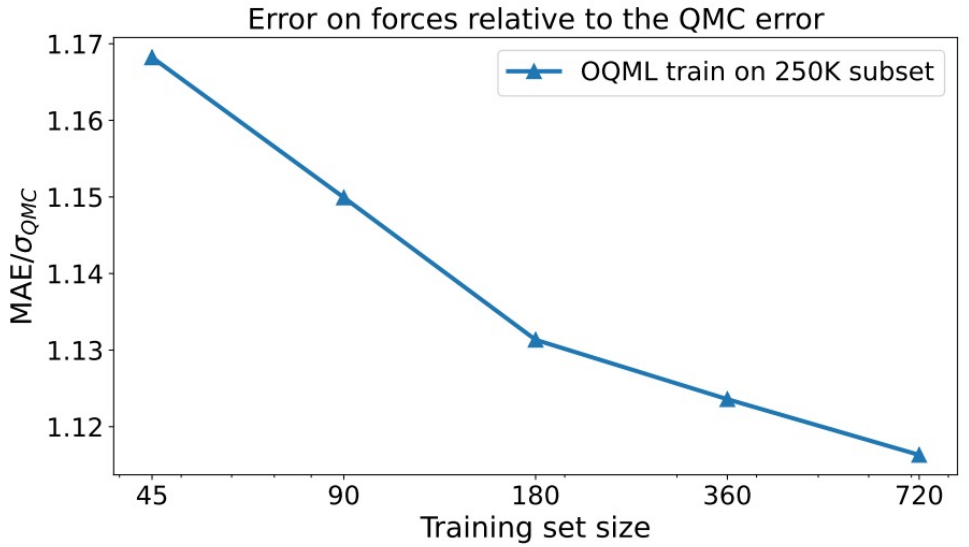
Symmetrized RDF $O_{(1,2)}$-H^+ from classic MD at **250K** (QMC vs DFT)



Machine Learning

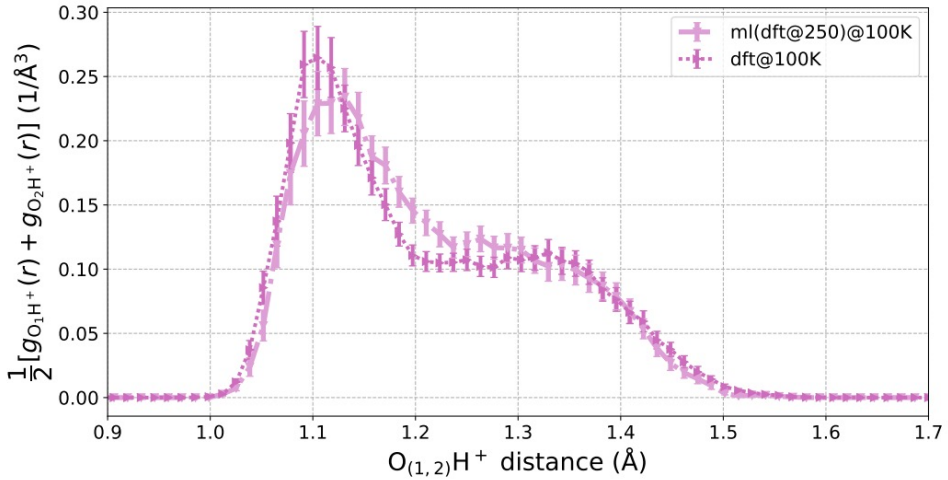
- FCHL19 representation
  (Local atomic environments)
- Training set extracted from MD
  configurations by farthest point sampling
- Operator Quantum Machine Learning
  (Kernel Ridge Regression like,
  with summation of local Gaussian kernel)



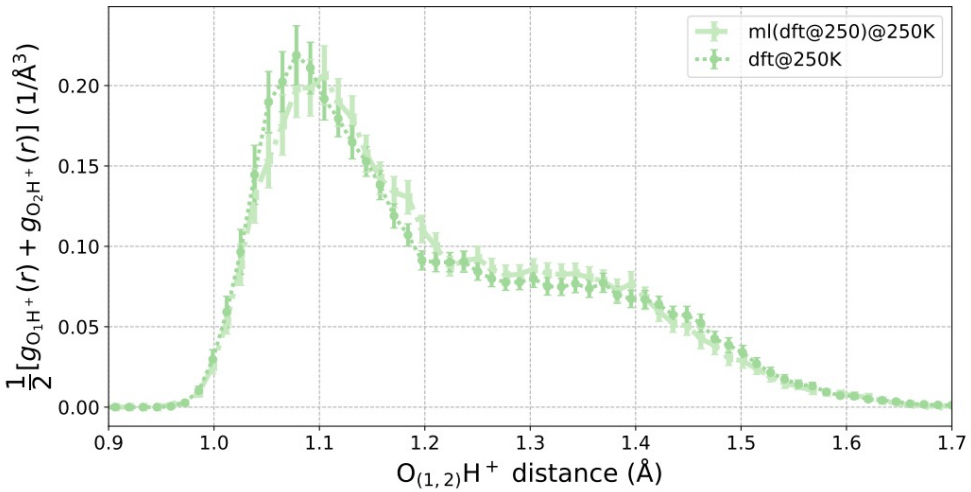


DFT vs ML(DFT) in OH+ RDF

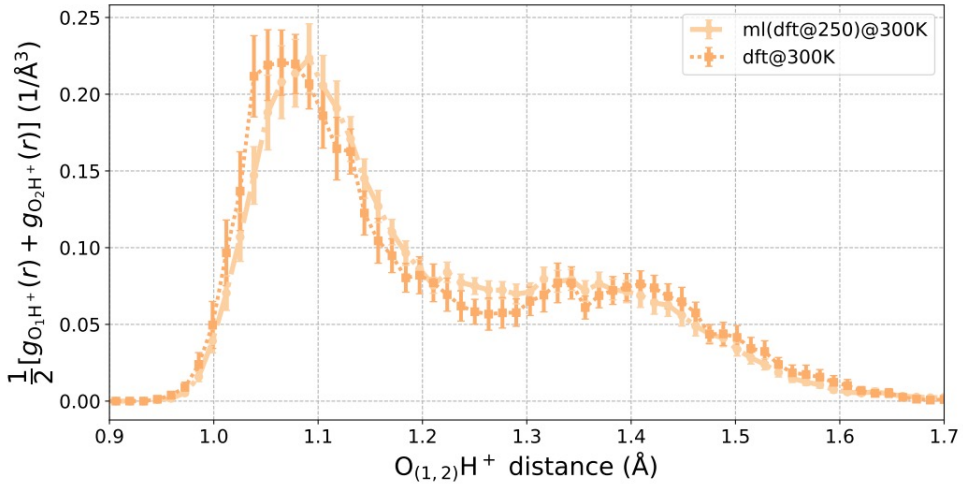
Symmetrized RDF $O_{(1,2)}$-H^+ from classic MD at **100K** (DFT vs ML)



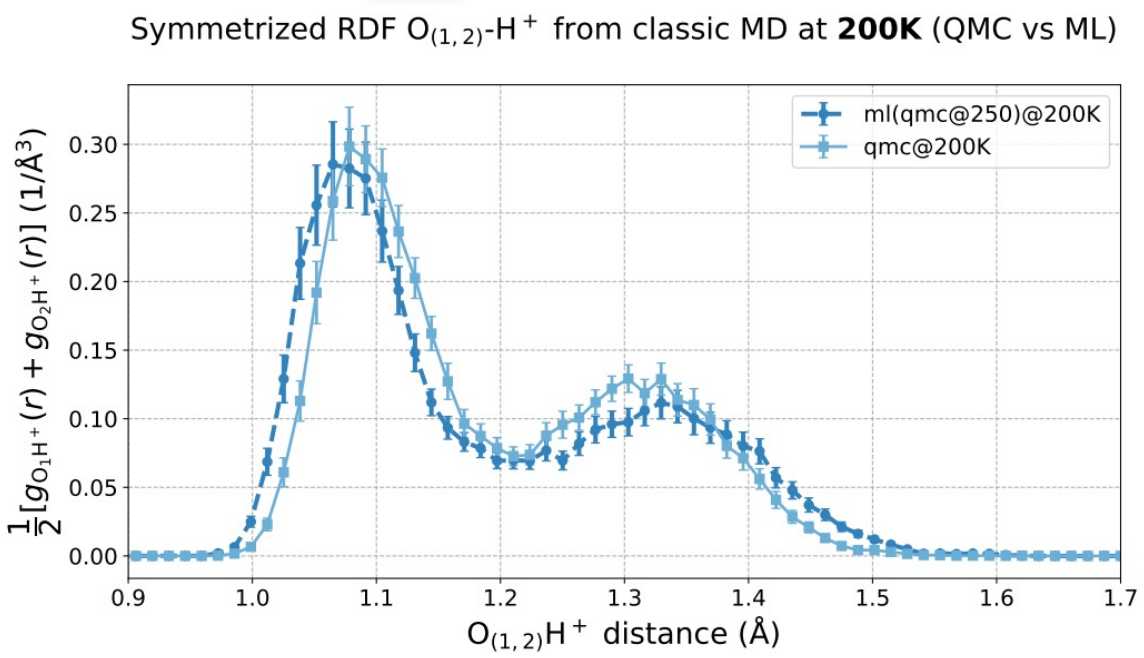
Symmetrized RDF $O_{(1,2)}$-H^+ from classic MD at **250K** (DFT vs ML)

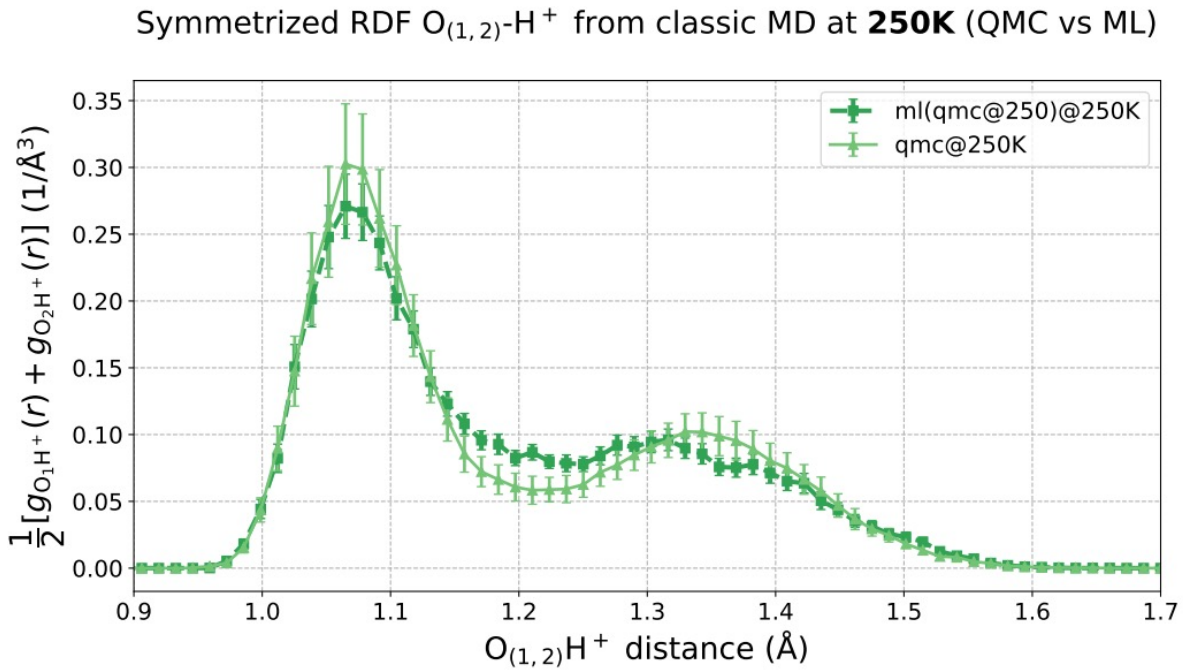


Symmetrized RDF $O_{(1,2)}$-H^+ from classic MD at **300K** (DFT vs ML)



QMC vs ML(QMC) in OH+ RDF





Perspectives

- Decrease QMC error bars
  on training set configurations (<0.004 Ha/au)
- Exploit quantum simulations, which are able to
  ”explore more” the shape of the barrier