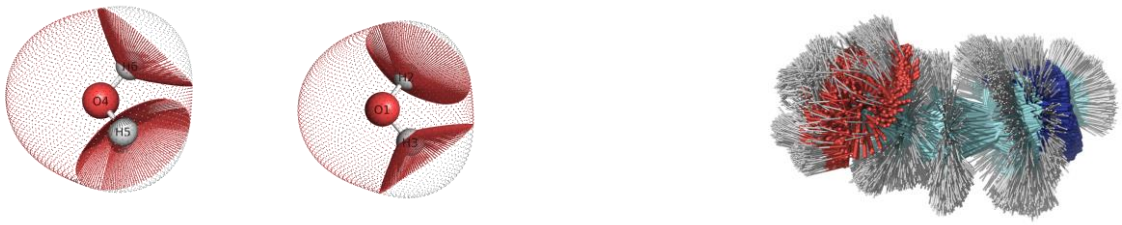
DL_FFLUX: A Machine-Learned Polarisable Force Field for Molecular Dynamics Simulations with Knowledgeable Atoms

Mohamadhosein Nosratjoo and Paul L.A. Popelier

Department of Chemistry, The University of Manchester, Oxford Road, Manchester M13 9PL, Great Britain

DL_FFLUX is a state-of-the-art force field that has been developed to make the idea of a universal force field a reality [1]. By its novel construct, DL_FFLUX "sees" the atoms and their electrons by utilising the quantum chemical topology (QCT) method. This results in quantum mechanically accurate **atomic** energies and multipole moments (MMs) in every step of an MD simulation. DL_FFLUX uses machine-learned models to predict these energies and flexible MMs [2]. A rather unique feature of this approach is that the machine learning does not carry out the atomic partitioning. Instead, QCT provides the atomic properties that are trained on, thereby guaranteeing their physical integrity. Our in-house FEREBUS [3] program is used to make models using the Gaussian Process Regression (GPR) method.



In this talk, the following questions will be answered:

1. Is it possible to have sub kcal/mol accuracy at speeds close to classical MD?
2. Can atoms be partitioned before machine learning?
3. Is it possible to have a non-bonded and non-parametrised force field?

References

[1] Symons, B.C., Bane, M.K. and Popelier, P.L.A, 2021. DL_FFLUX: a parallel, quantum chemical topology force field. *Journal of Chemical Theory and Computation*, *17*(11), pp.7043-7055.

[2] Symons, B.C. and Popelier, P.L.A., 2022. Flexible multipole moments in smooth particle mesh Ewald. *The Journal of chemical physics*, *156*(24).

[3] Burn, M. J.; Popelier, P. L. A., FEREBUS: a High-performance Modern Gaussian Process Regression Engine. Digital Discovery 2023, 2, 152-164.