Contribution ID : **121** Type : **Poster Presentation**

EuCompChem2025 – Matthew Brown – Oral

Machine learning potentials (MLPs) aim to bridge the gap between force fields and ab initio methods, allowing for accurate calculations with a reduced computational cost. This capability promises to benefit several research areas. For example, in crystal structure prediction, highly accurate methods are required to capture small energy differences between different crystal structures [1]. In the determination of protein structures MLPs offer an opportunity to improve upon calculations with traditional force fields which generally lack consistency [2].

FFLUX [3,4] force fields use Gaussian process regression (GPR) models trained on data from quantum chemical topology (QCT) calculations to predict intramolecular (or intra-system) energies and multipole moments up to the hexadecapole moment. These models allow for fully flexible molecules with geometry dependent electrostatic interactions. In previous studies focussing on liquid water [5], formamide polymorphs [6] and gas phase clusters [7,8], dispersion and repulsion have been represented by Lennard-Jones potentials.

Within our workflow, intermolecular interactions can be machine learned using the same QCT/GPR methodology, bringing FFLUX force fields closer to quantum mechanics. This talk highlights ongoing work to remove the need for external potentials such as the Lennard-Jones potential in our simulations. GPR models trained on clusters allow intermolecular repulsion to be modelled as well as intermolecular polarisation allowing for greater accuracy in calculations.

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