UNIVERSITÄT DUISBURG ESSEN

Offen im Denken

Theorie-Kolloquium SS 2023
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Bespoke Interaction Potentials for Computer-Aided Drug Design

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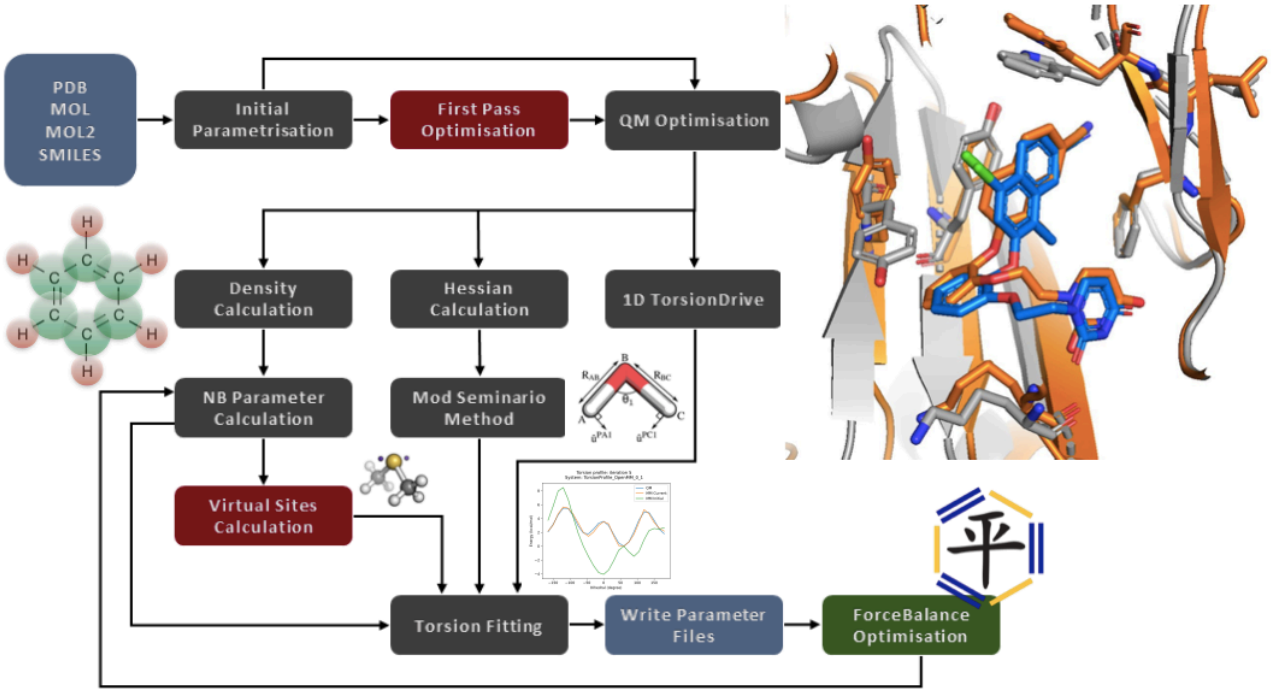

Drawing on computational methods that include atoms-in-molecule electron density partitioning and machine learning, I will describe some of our efforts to design accurate, automated and bespoke inter- and intramolecular potentials, with a view to applications in condensed phase atomistic modeling and computer-aided drug design.
I will give an overview of our force field derivation software, QUBEKit, which is able to generate bespoke charge, Lennard-Jones and virtual site parameters directly for the molecule under study [1]. Furthermore, I will explain how recent collaborations with the Open Force Field Initiative enable the parameterisation of charge and long-ranged interactions for graph neural network potentials and the derivation of transferable force fields with advantageous functional forms [2] that work in the condensed phase.
Finally, I will describe ongoing efforts to train and implement future machine learning based potentials, including the Atomic Cluster Expansion force field, in the OpenMM package for computer-aided drug design applications [3].

[1] Ringrose, C., et al. (2022). Phys Chem Chem Phys, 24, 17014-17027
[2] Horton, J., et al. (2023). ChemRxiv, 10.26434/chemrxiv-2023-28r9s
[3] Kovács, D., et al. (2021). J. Chem. Theory Comput., 17, 7696-7711