SIMULATION OF METAL COORDINATION COMPLEXES WITH THE BuRNN APPROACH

Bettina Lier[a], Peter Poliak[a,b], Philipp Marquetand[c], Julia Westermayr[d,e*] and Chris Oostenbrink[a*]

[a]Institute of Molecular Modeling and Simulation, University of Natural Resources and Life Sciences, Vienna, Austria
[b]Institute of Physical Chemistry and Chemical Physics, Slovak University of Technology in Bratislava, Bratislava, Slovakia
[c]Institute of Theoretical Chemistry, University of Vienna, Vienna, Austria
[d]Wilhelm-Ostwald-Institute for Physical and Theoretical Chemistry, University of Leipzig, Leipzig, Germany
[e]Center for Scalable Data Analytics and Artificial Intelligence (ScaDS.AI), Dresden/Leipzig, Germany

Metal sites and coordinate bonds represent a major challenge for classical molecular mechanics (MM) simulations, complicating force field parameterization and therefore often require a full quantum mechanical (QM) description. However, pure QM simulations remain intractable for large systems. Instead, they can be simulated by hybrid QM/MM methods. Partitioning the system into two regions that are treated at different levels of theory, though, comes with various artifacts.

In this talk we will introduce BuRNN, a Buffer Region Neural Network approach as an alternative to conventional QM/MM schemes [1]. It utilizes a buffer region between the QM and MM region, which is treated at both levels of theory. Within the buffer, the interactions are therefore a combination of MM interactions and the effect of the QM region on the electronic degrees of freedom. This requires a second QM calculation, such that the buffer can experience full electronic polarization due to the QM region. Thus, artifacts at the interface largely cancel in the difference. To avoid excessive computational costs, we employ atomistic neural networks (NN). The performance of the method is demonstrated using the hexa-aqua iron complex as a model system, which shows that BuRNN can be applied for metal-ligand interactions.

[1] Lier, B., Poliak P., Marquetand, P., Westermayr J. & Oostenbrink, C. *J. Phys. Chem. Lett.* 13, 3812–3818 (2022)