4th live session of **Focus Materialchemie** – Wednesday, **26.04.2023** 16:00 – @ **Seminarraum Lehar 01** (TU-Wien, Getreidemarkt 9, BC, OG. 01, room A46) – join us on **ZOOM** (ID: 983 0066 2349)

Van der Waals interactions in neural-networks

Nina Buckova[a]

[a]*Institute of Materials Chemistry, Technische Universität Wien (TU Wien), Getreidemarkt 9, Vienna, Austria*

In recent years, new methods, based on machine-learning techniques and neural networks, have been developed to calculate the thermodynamic and spectroscopic properties of various systems with high precision and low computational costs. However, current neural-networks have a significant limitation: they only take local short-range interactions between atoms and molecules into account, and largely ignore the long-range interactions that may strongly influence the properties of materials. This limitation may have significant consequences for predicting the physical properties of materials that are primarily determined by such long-range interactions. Using water as a case study, this contribution will discuss the extent to which long-range dispersive interactions can be taken into account in our neural-network NeuralIL, and how limitations affect the accuracy of predicted physical properties.