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)

Electrostatic Interactions in Neural-Network Force Fields

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Neural-network force fields provide a computationally efficient, flexible and transferable way to compute forces and further quantities with ab-initio-like accuracy, for example for use in high-throughput applications. Such models often work in part by encoding the absolute coordinates using descriptors which capture the immediate environment of an atom. These are in most cases defined via a cutoff radius, making them local by definition. While such networks already produce excellent results using these descriptors, an accurate modelling of long-range interactions is desirable to move towards more physical and transferable models of the systems of interest.

In the present work, a methodology to model electrostatic interactions using a neural-network force field has been developed. Training data that represents only the electrostatic interactions between the atoms in the system is generated via Density Functional Theory calculations. Formal charges, which provide further information to the model, are predicted using a second, supporting, electron-passing neural-network. The applicability of the approach is demonstrated on surface reconstructions and liquids.