Extra Session of Focus Materialchemie – Tuesday, **05.11.2024** 16:00
@ BA0156A (TU-Wien, Getreidemarkt 9, BA, OG. 01, room A56)

Atomistic Modelling of Structure Formation and Phase Transitions in Si-Ox Compounds using Machine-Learning Interatomic Potentials

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Silica is used in a wide range of applications from catalysis to construction to microelectronics. The related silicon monoxide is promising for applications as an anode material in lithium batteries. Although these materials have been extensively studied for more than a century, there are still many open questions. For example, the high-pressure transformations of silica are not fully understood. Moreover, in the case of silicon monoxide, there is not even an atomistic structure model that captures the complexity of the structure. In this talk, I will show how we have used machine-learning interatomic potentials combined with atomistic modelling to investigate these problems. First, I will show how active learning combined with large-scale molecular dynamics simulations can be used to generate a comprehensive density-functional theory dataset for this complex system [1,2]. I then show how well the machine-learning potential based on this database reproduces the thermodynamics of the system. Finally, I show two applications of the model: (1) We have studied in detail the phase transitions of quartz under high-pressure compression and explain why different experimental results are obtained depending on the exact boundary conditions [3,4]. (2) I present structural models of the amorphous structure of silicon monoxide that are consistent with experimental observations and may also pave the way for experimental tuning of this structure [2].

[1] L. C. Erhard et al., *npj Comput Mater* **8**, 90 (2022) https://doi.org/10.1038/s41524-022-00768-w.

[2] L. C. Erhard et al., *Nat Commun* **15**, 1927 (2024). https://doi.org/10.1038/s41467-024-45840-9.

[3] L. C. Erhard et al., *Modelling Simul. Mater. Sci. Eng.* **32** ,065029 (2024), https://doi.org/10.1088/1361-651X/ad64f3

[4] L. C. Erhard et al., arXiv:2406.17676, https://doi.org/10.48550/arXiv.2406.17676