UNIVERSITÄT LEIPZIG

Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie

How Molecular-Level Modeling and Machine Learning Can Accelerate the Discovery of Nanoporous Materials

Kolloquium zur Theoretischen Chemie mit

Prof. Randall Q. Snurr (Northwestern University)

12.09.2022

17.00 Uhr

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Abstract:

Metal-organic frameworks (MOFs) are a versatile class of nanoporous materials synthesized in a "building-block" approach from inorganic nodes and organic linkers. By selecting appropriate building blocks, the structural and chemical properties of the resulting materials can be finely tuned, and this makes MOFs promising materials for applications such as gas storage, chemical separations, drug delivery, and catalysis. Because of the predictability of MOF synthetic routes and the nearly infinite number of possible structures, molecular modeling is an attractive tool for screening new MOFs before they are synthesized, and methods from data science are finding increasing application in this field. This talk will discuss how molecular-level modeling and machine learning can accelerate the computational discovery of new MOFs for particular applications.

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