Frontier Chemistry Center
フロンティア化学教育研究センター

講演会

演 題：**From Machine-Learning Interatomic Potentials to Materials Chemistry**

講 師：**Dr. Volker L. Deringer**

University of Cambridge, the U.K.

日 時：2019 年 8 月 2 日（金）14:45～15:45

場 所：工学部材料・化学棟小会議室（MC527）

要 旨：

Understanding the links between structure and properties in materials is one of the most central challenges for chemistry. Atomic-scale simulations based on density-functional theory (DFT) have played important roles in this – but they are computationally expensive and can describe structurally complex materials only in small model systems. Novel simulation methods based on machine learning (ML) have recently attracted a lot of attention in computational physics, chemistry, and materials science: by “learning” from reference DFT data, they achieve similar accuracy but require only a small fraction of the cost.

In the first part of this talk, I will argue that ML-based interatomic potentials are particularly useful for studying structurally complex materials, such as amorphous (non-crystalline) solids. I will describe an ML potential for amorphous carbon [1] that was built using the Gaussian Approximation Potential (GAP) framework [2], with a special view on what is needed to create and validate ML potentials for the amorphous state. I will present recent applications of GAP-ML models to porous and partly "graphitised" carbons that are relevant for batteries and supercapacitors [3], and to amorphous silicon, where ML-driven simulations allowed us to unlock long simulation times and accurate atomistic structures [4]. In the second part, I will point out possible directions for the automated exploration and “learning” of solid-state potential-energy landscapes. We recently introduced an ML-driven approach to inorganic crystal structure prediction, dubbed GAP-driven random structure searching (GAP-RSS) [5]. This technique, iteratively exploring and fitting structural space, allowed us to create to a flexible and accurate interatomic potential for elemental boron [5], and more recently to develop a more general computational framework that can explore and fit potential-energy surfaces for different materials [6]. These early results are hoped to enable a more widespread use of ML-driven materials simulations in the years to come.

References: [1] Phys. Rev. B 2017, 95, 094203, [2] Phys. Rev. Lett. 2010, 104, 136403, [3] Chem. Commun. 2018, 54, 5988, [4] VJ. Phys. Chem. Lett. 2018, 9, 2879, [5] Phys. Rev. Lett. 2018, 120, 15600, [6] arXiv:1905.10407.

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