Contribution ID: **21** Type: **Contributed Talk (15 min)**

Learning Conductance: Gaussian Process Regression for Molecular Electronics

Wednesday, 21 September 2022 10:00 (15 minutes)

Experimental studies of charge transport through single molecules often rely on break junction setups, where molecular junctions are repeatedly formed and broken while measuring the conductance, leading to a statistical distribution of conductance values.
Modeling this experimental situation and the resulting conductance histograms is challenging for theoretical methods, as computations need to capture structural changes in experiments, including the statistics of junction formation and rupture.

This type of extensive structural sampling implies that even when evaluating conductance from computationally efficient electronic structure methods, which typically are of reduced accuracy, the evaluation of conductance histograms is too expensive to be a routine task.
Highly accurate quantum transport computations are only computationally feasible for a few selected conformations and thus necessarily ignore the rich conformational space probed in experiments.

To overcome these limitations, we investigate the potential of machine learning for modeling conductance histograms, in particular by Gaussian process regression. We show that by selecting specific structural parameters as features, Gaussian process regression can be used to efficiently predict the zero-bias conductance from molecular structures, reducing the computational cost of simulating conductance histograms by an order of magnitude.
This enables the efficient calculation of conductance histograms even on the basis of computationally expensive first-principles approaches by effectively reducing the number of necessary charge transport calculations.
We also provide an outlook how techniques such as active learning can be used to push the boundaries of Machine Learning approaches.

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Session Classification: Molecular Structure Analysis

Track Classification: Molecular Structure Analysis