Advances in machine learning for SPM analysis and structure search

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Recent years have displayed an exponential growth in the development of machine learning tools in image and data analysis, automation and optimization of experiments, as well as computational modeling. In our group, we are actively researching new methods and combinations thereof relating to each of the aforementioned categories.We have recently demonstrated the potential of neural network-based geometry prediction tools on AFM and STM images.[1][2] Also, we have shown how suitable training data can be generated with the probe particle model [3] on plausible structures obtained using machine learning interatomic potentials.Furthermore, we are taking advantage of the rapid energy evaluations provided by these potentials in exploring accelerated structure search methods, such as Bayesian optimization and minima hopping.[4] While selective chemical reactions induced by the SPM tip has been achieved in the past, there are currently no reports on their automation, much due to the highly complex parameter space. We are employing reinforcement learning to acquire the molecule manipulation parameters to selectively break C-Br bonds, providing the first example of its kind.

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[4] Joakim S. Jestilä, Nian Wu, Fabio Priante, and Adam S. Foster, *J. Chem. Theory Comput.* **20, 5**, 2297–2312 (2024).