Autonomous chemical reactions in scanning tunneling microscopy

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Several breakthrough studies have harnessed scanning probe microscopy (SPM) manipulations to control chemical reactions in on-surface molecular synthesis [1, 2, 3]. In general, for scanning tunnelling microscope (STM) manipulations, they are predominantly controlled via parameters of the tip position, pulse voltages and tunneling conductance. However, the selection of proper parameters requires extensive domain knowledge, which is time consuming and not necessarily transferable to new systems. Recent research has allowed the automation of a wide range of challenges in SPM, including image quality assessment, lateral and vertical manipulation [4, 5, 6]. However, the automation for breaking or forming covalent bonds, which is an indispensable step during chemical synthesis is, as yet, unexplored. To address this problem, we developed our deep reinforcement learning (DRL) approach to automate bromine removal from 5,15-bis(4-bromo-2,6-methyl-phenyl)porphyrin (Br2Me4DPP) through learning manipulation parameters in STM. Meanwhile, DFT calculations were implemented to explore the reaction mechanism in combination of STM results and DRL results.

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