Obtain physical insights into molecule-substrate interactions using AI-controlled manipulations via Scanning Tunneling Microscopy

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Motivation

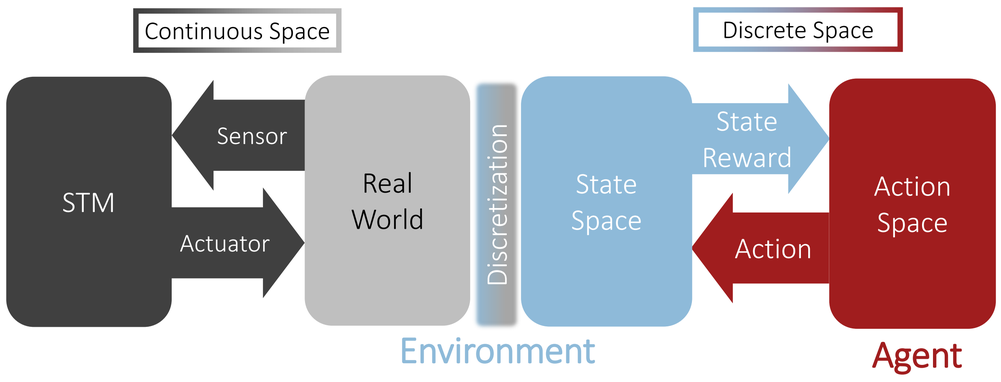
Challenge: Moving and re-orienting molecules on a surface with high reliability is non-trivial and difficult to achieve. The interaction process is non-intuitive and therefore the outcome of an action is hard to predict.

Goal: Constructing molecular nanostructures by arranging and orienting molecules at will. This will lead to physical insight into molecule-molecule and molecule-substrate interactions.

Approach: An Artificial Intelligence is used to learn molecular manipulations by interacting with the molecule and achieve certain objectives.

Reinforcement Learning

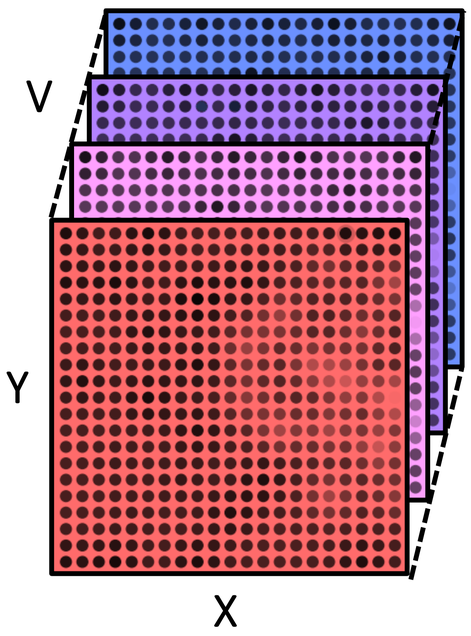
Reinforcement learning is mapping *states* to *actions*

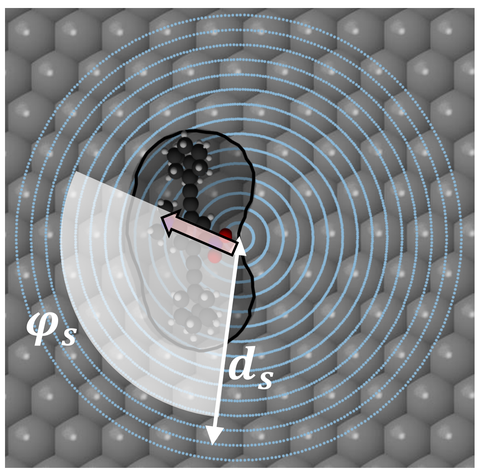


Actions are judged by the *Reward R*

Enables the learning of tasks in changing environments

Action Space	State Space
Tip-positions (X_a, Y_a) and bias voltages V_a	Angles φ_s between dipole orientation and goal direction
	Distance d_s between molecular pivot point and goal position

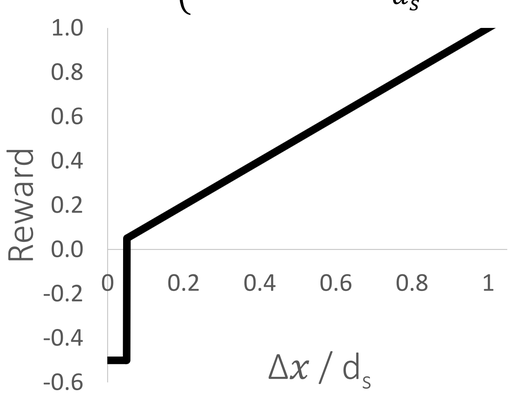




Reward

The *reward* dictates the behavior of the agent

$$R(\Delta x) = \begin{cases} -1 & , \Delta x < d_{min} \\ \dfrac{\Delta x}{d_{s\_max}} & , d_{min} < \Delta x \; and \; \dfrac{\Delta x}{d_{s\_max}} \leq 1 \\ 1 & , \dfrac{\Delta x}{d_s} > 1 \end{cases}$$



Difference in goal distance between two successive timesteps

$$\Delta x = d_t - d_{t+1}$$

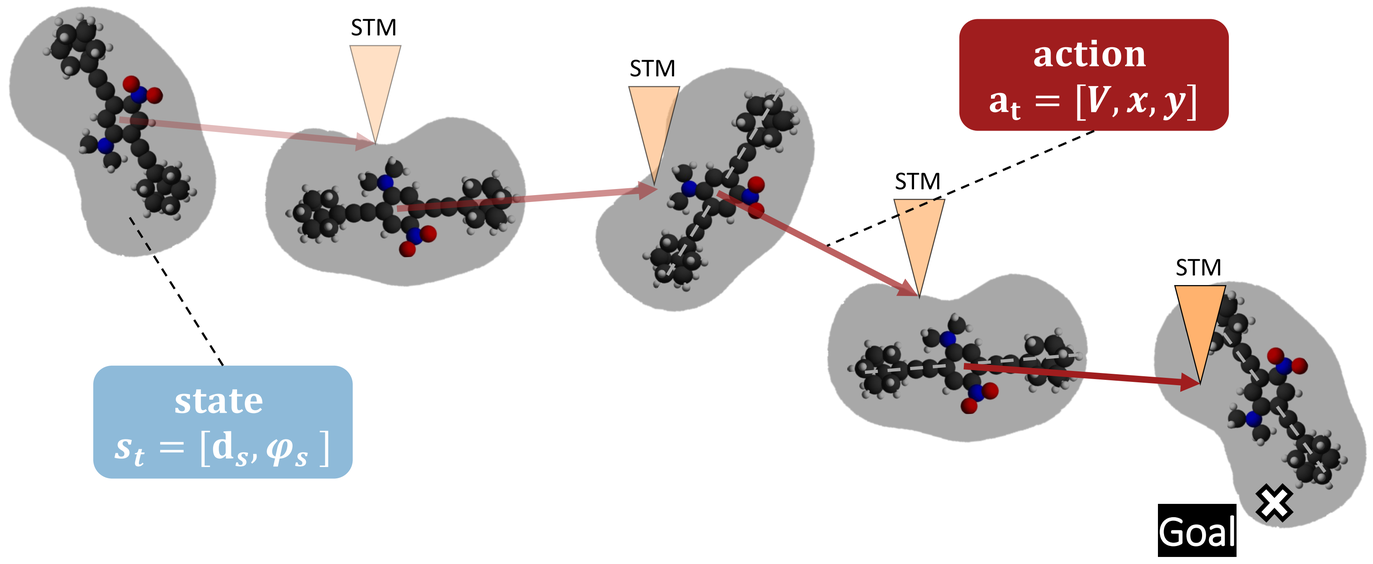
Encourages the agent to manipulate the molecule precisely towards the goal

Design of the Artificial Intelligence

Design of the Environment

Manipulate molecule along a predefined race-track

No contact required



The Q-Learning Algorithm

Q-Learning is an off-policy temporal difference (TD)-control algorithm

$$\mathbf{Q^{new}}(\mathbf{s_t}, \mathbf{a_t}) \leftarrow \mathbf{Q}(\mathbf{s_t}, \mathbf{a_t}) + \boldsymbol{\alpha}\left(\mathbf{R_{t+1}} + \boldsymbol{\gamma} \max_{\mathbf{a}} \mathbf{Q}(\mathbf{s_{t+1}}, \mathbf{a}) - \mathbf{Q}(\mathbf{s_t}, \mathbf{a_t})\right)$$

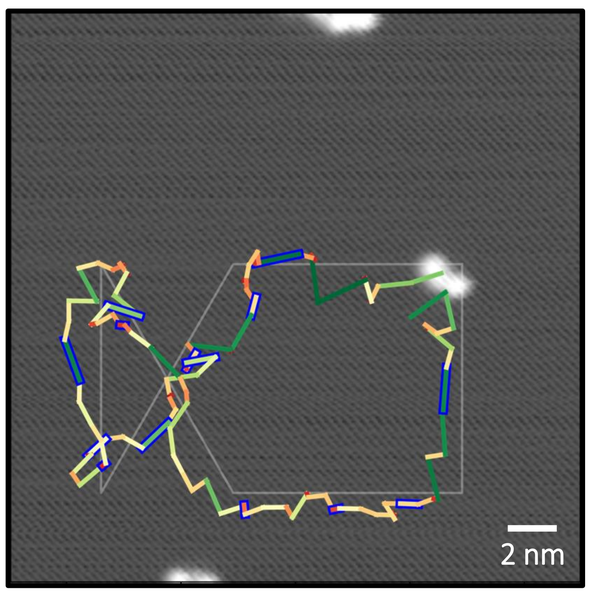
ε-greedy strategy:

- Exploration: select actions based on highest uncertainty of Gaussian Process Regression

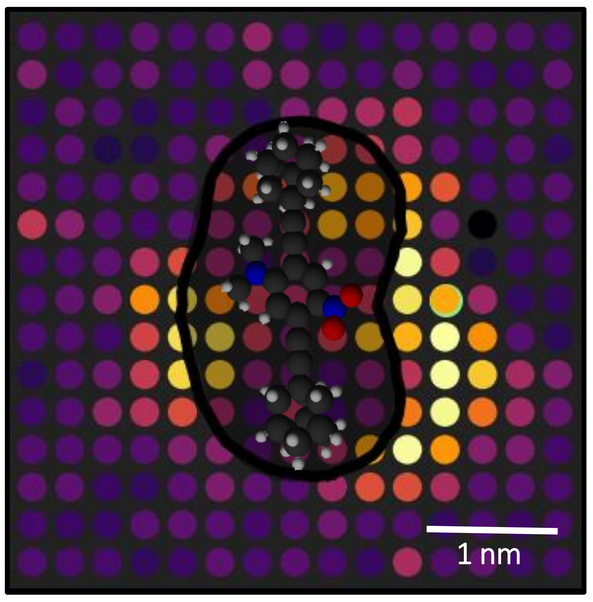
- Exploitation: select best-known action

Results

1. Artificial Intelligence maneuvers molecule along a trajectory

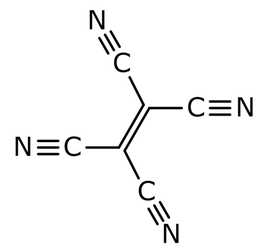


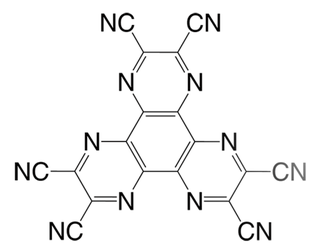
2. Gain physical insights of tip-molecule interactions



Outlook

Study the diffusion and transition rates for of TCNE/Cu and HATCN/Ag





Contact

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