Efficient and Safe Molecular Assembly via Reinforcement Learning and Constraint Solving

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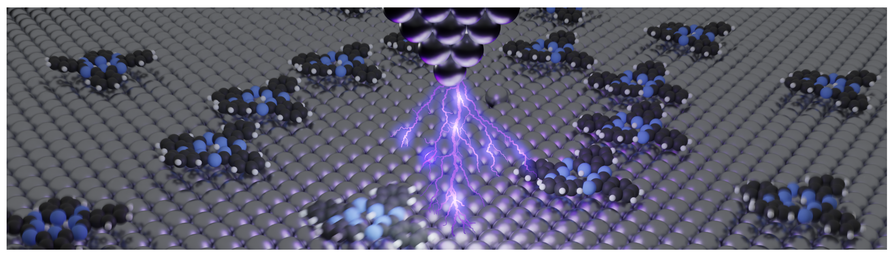
The Challenge: Autonomous Molecular Assembly



Scanning tunnelling microscopy (STM) enables sub-nanometre manipulation of individual atoms and molecules — creating quantum corrals, logic circuits, and novel nanostructures.

Molecules and obstacles are randomly distributed on a substrate ⇒ the goal is to arrange the molecules into a target structure, which needs an operator to:

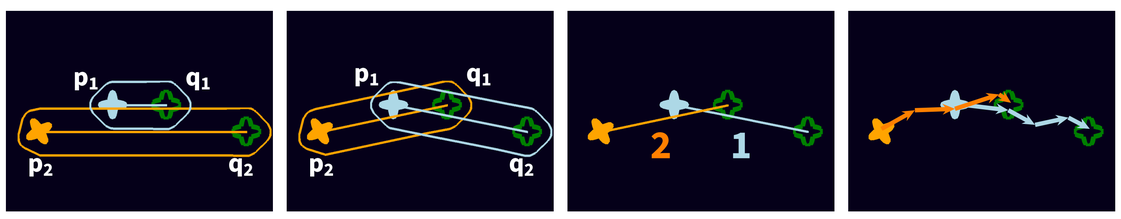
- **Discover** molecule-specific responses to tip actions
- **Plan** when and where to move each molecule
- **Execute** hundreds of precise tip manipulations by hand

Human experts spend months constructing assemblies of ∼100 atoms.

⇒ **We build the first autonomous framework for molecular assembly.**

Our Approach: Two-Phase Autonomous Assembly

Our approach uses Satisfiability Modulo Theories (SMT) solving to find a schedule that allows each molecule to be moved within an empty corridor. Policies trained using Reinforcement Learning (RL) then execute the low-level manipulations.

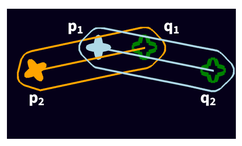


(a) No feasible schedule possible ⇒ conflict (b) Matching with resolved conflicts (c) Collision-free schedule (d) RL agents execute computed plan

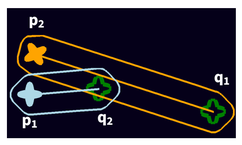
- **Phase 1** — assign molecules to targets; use SMT to find a collision-free execution order; resolve conflicts and repeat.
- **Phase 2** — RL agents steer each molecule through its corridor to the target in schedule order.

Phase 1: Collision-Free Assembly Planning

- **Hungarian matching** — compute assignments `Match` of molecule-target pairs a_{ij}, minimising total travel distance
- **Precedence constraints** — corridors that overlap induce ordering constraints, collected in `Cons`
- **SMT scheduling (Z3)** — find ordering satisfying `Cons`; if unsatisfiable, set distance of conflicting pairs a_{ij} to ∞ and recompute `Match`



(a) Start precedence constraint



(b) Target precedence constraint

Figure: Precedence Constraints

SMT formula: Each $a_{ij} \in$ `Match` gets a unique schedule slot s_{ij}, ordered to respect all constraints in `Cons`.

$$\varphi = \bigwedge_{\substack{a_{ij},a_{kl}\in\texttt{Match},\\ a_{ij}\neq a_{kl}}} s_{ij} \neq s_{kl} \wedge \bigwedge_{(a_{ij},a_{kl})\in\texttt{Cons}} s_{ij} < s_{kl}.$$

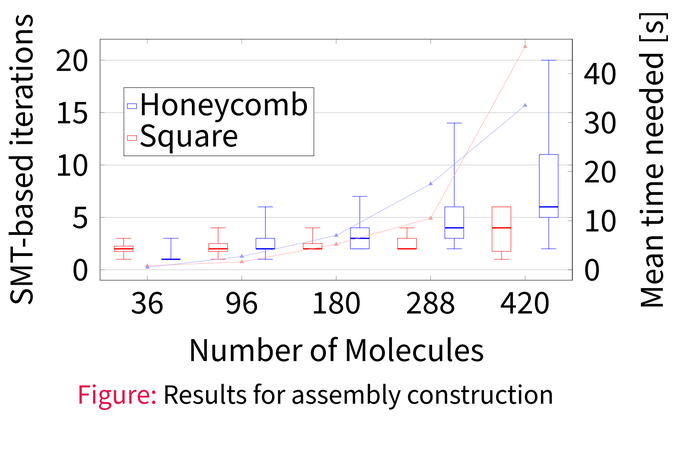


Figure: Results for assembly construction

Phase 2: RL Agents for Molecule Manipulation

Probabilistic molecule responses to STM tip actions are modelled as an MDP. RL agents learn to steer each molecule to its target within the assigned corridor.

MDP Formulation:

- *State:* molecule position and orientation; target position and orientation
- *Actions:* tip placement relative to molecule center
- *Reward:* $\mathcal{R}_{\text{move}}$ progress toward target
  $+ \mathcal{R}_{\text{corr}}$ corridor adherence
  $+ \mathcal{R}_{\text{rot}}$ orientation alignment

We train policies using **PPO**, **TQC**, and **CrossQ** for three different types of molecules and use the best performing per type.

Molecule	Corridor Adherence	Mean movement
Circular	99.7%	0.83 nm
Cross (low var.)	99.8%	0.73 nm
Cross (high var.)	97.3%	0.63 nm

End-to-End Autonomous Assembly

We evaluate the complete pipeline on different assemblies with up to **420 molecules**. Across 165 assembly runs, over **30 000** molecules were manipulated with only 10 collisions observed.

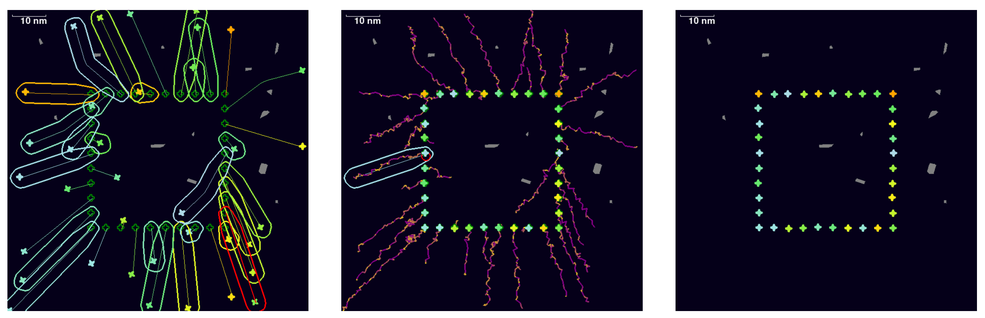


Figure: Complete approach for a square with 36 molecules

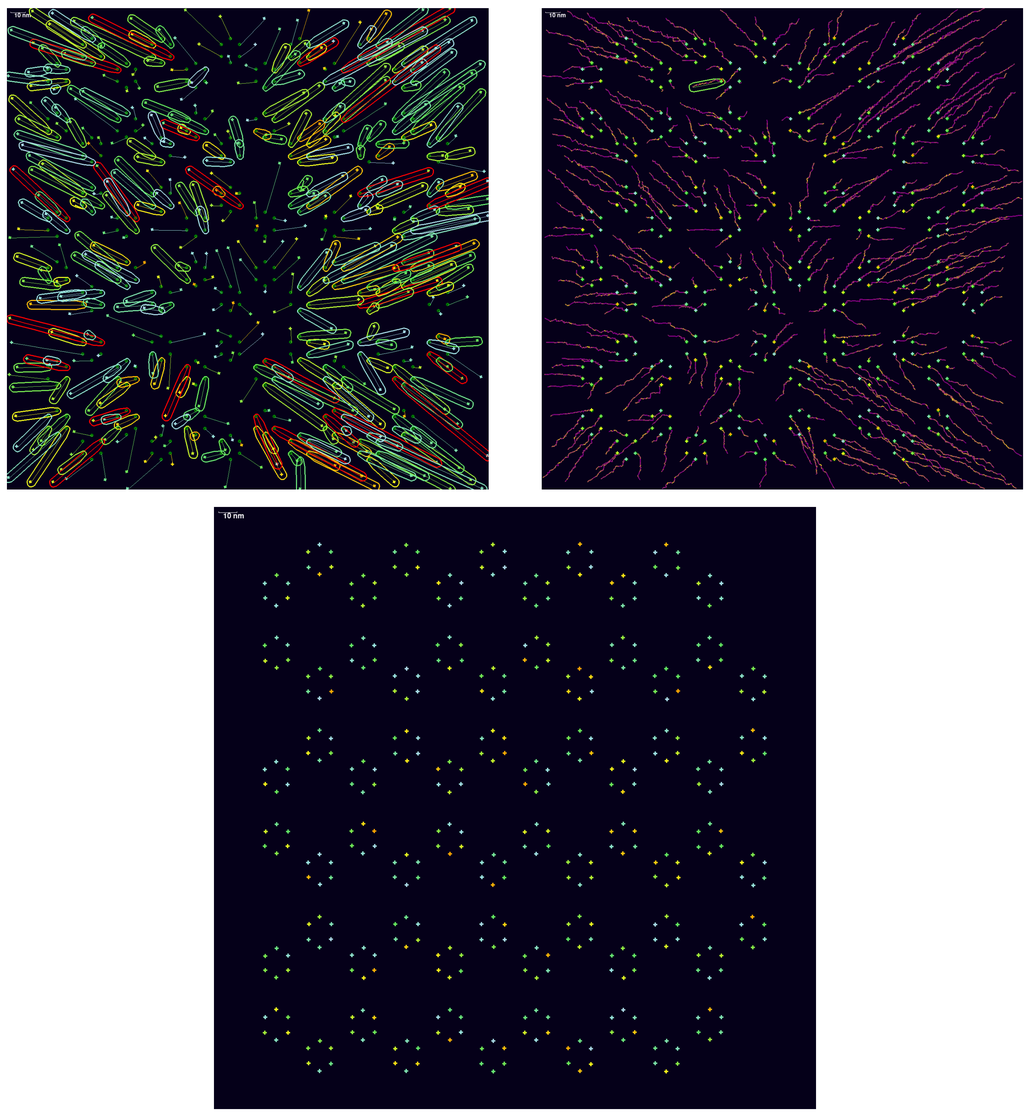


Figure: Complete approach for a *honey comb* structure with 420 molecules

Conclusion

Contributions:

- First autonomous framework for **molecular** assembly using scanning tunnelling microscopy
- SMT-based planning scales to hundreds of molecules
- RL agents execute low-level manipulations

NanoAssemblyGym:

- STM simulator for RL training and assembly planning

Next: Close Sim-to-Real Gap:

- Tip-change detection and recovery
- Richer STM actions

Takeaway: SMT planning + RL control enable scalable, collision-aware molecular assembly.

Code:

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