N-heterocyclic carbene adsorption and self-assembly on Au(111): Fine-tuning the binding mode

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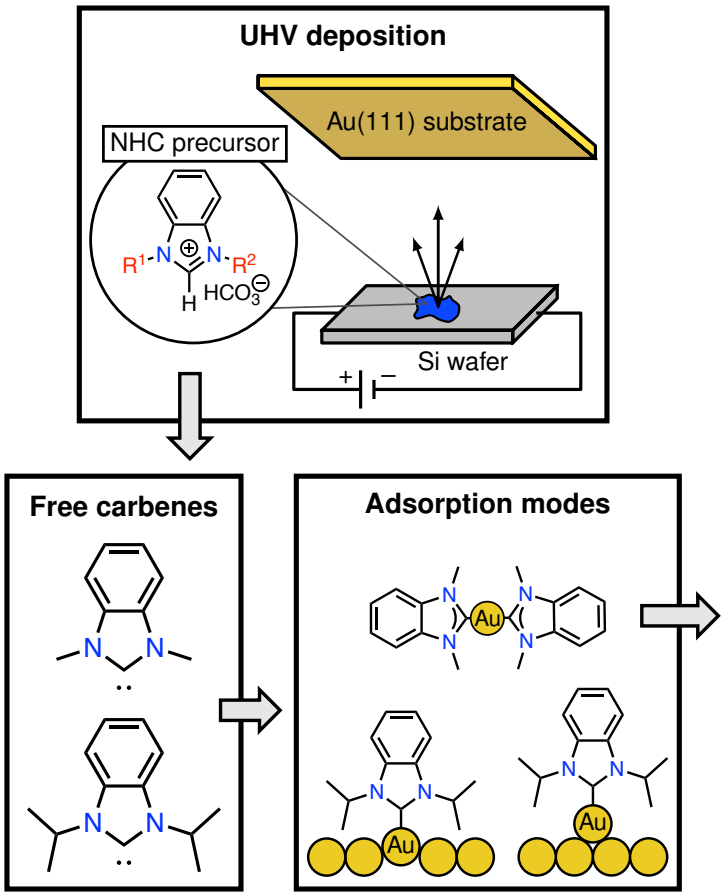
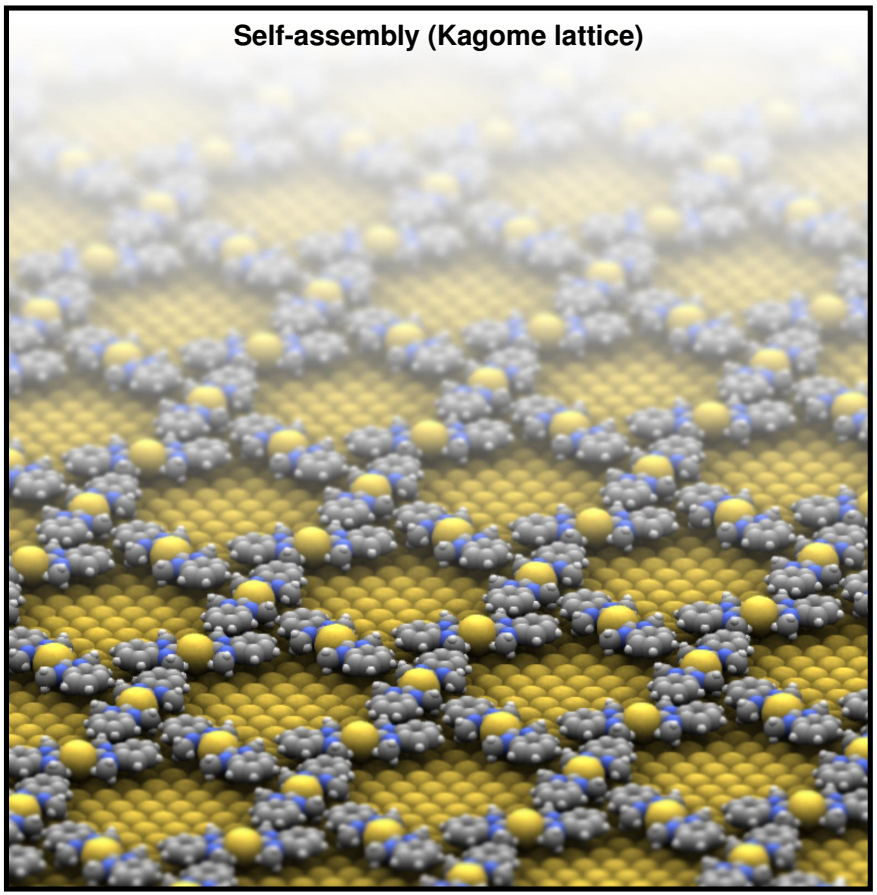
N-heterocyclic carbenes (NHCs)

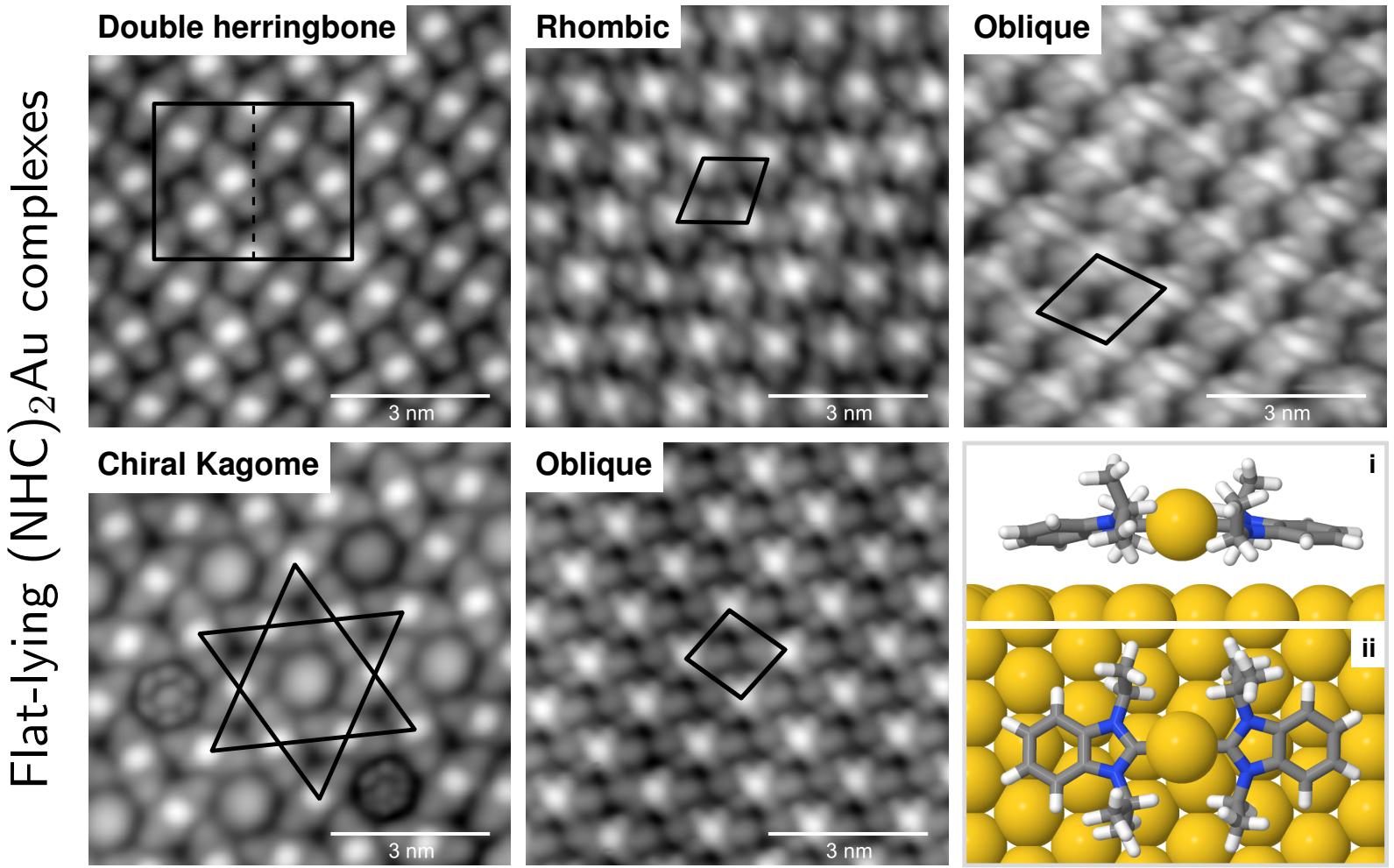
- Scanning tunnelling microscopy (STM) study of NHC-based self-assembled monolayers (SAMs)





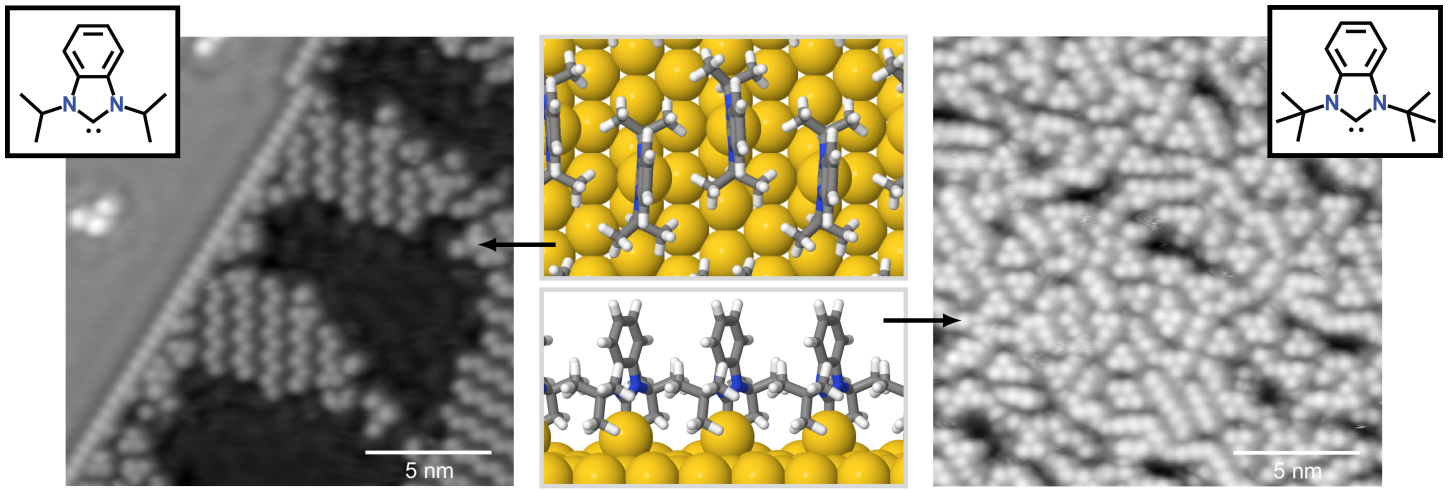
Flat-lying NHC SAMs

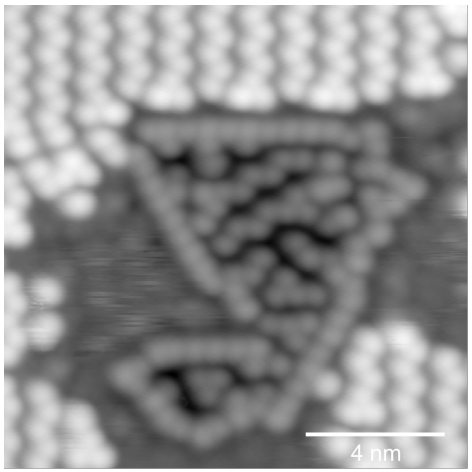
- SAMs prepared on room-temperature Au(111) surfaces



Upright NHC SAMs

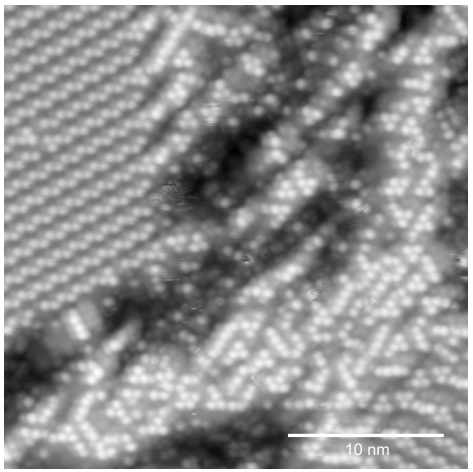
- NHCs with bulkier wingtip groups (*i*Pr, *t*Bu) stand upright on adatoms





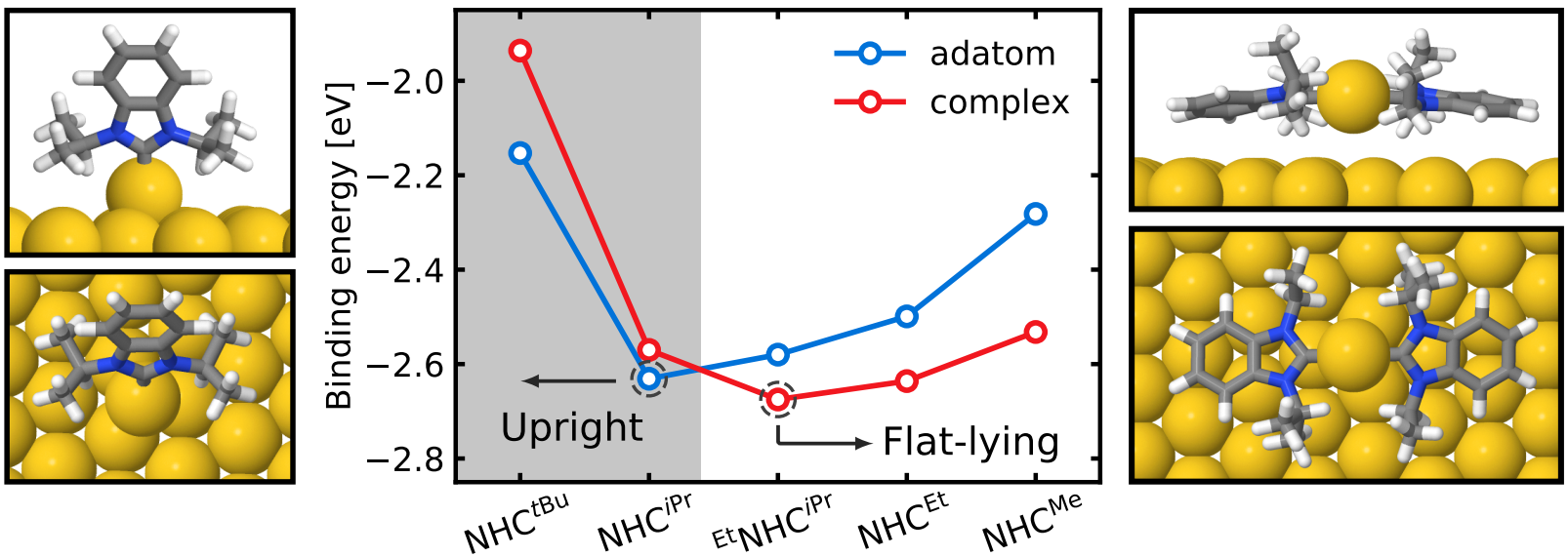
Experimental evidence includes

- Vacancy islands
- Lattice structure
- Co-deposition experiment
- Apparent height comparison at steps



Comparison with density functional theory (DFT)

- Experimental observations consistent with *ab initio* DFT calculations



- Fine-tuning of the wingtip substituents provides flexibility in controlling the binding mode
  - Surface coverage and substrate temperature are also critical factors (see video presentation!)

Acknowledgements

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- **My group (STM)**
  Queen's Physics
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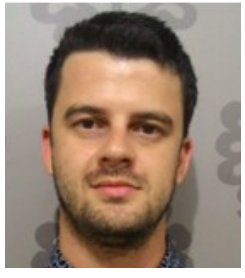
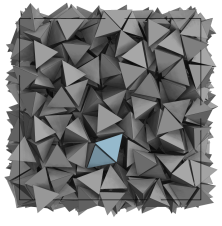
  - Greg van Anders





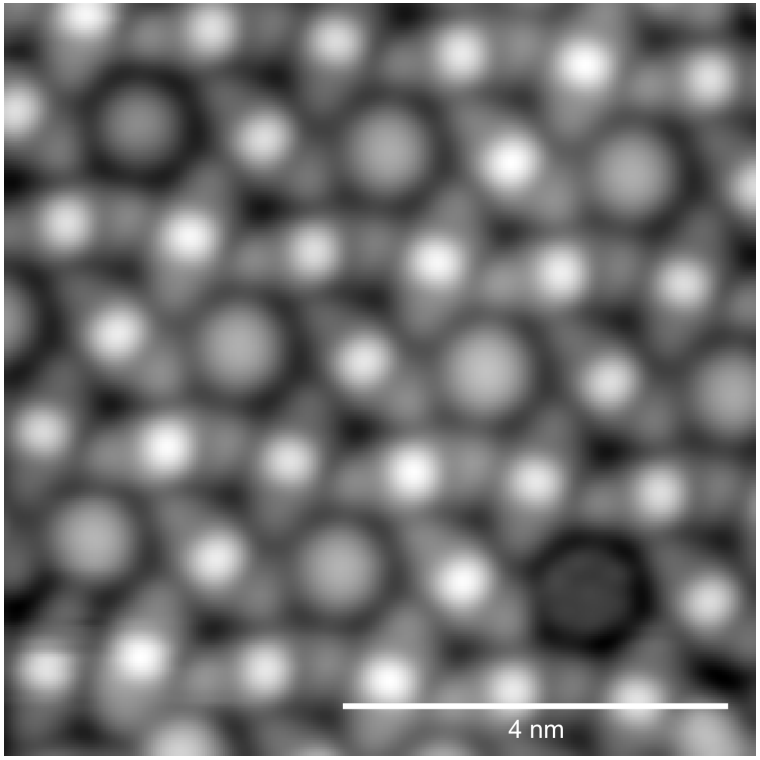



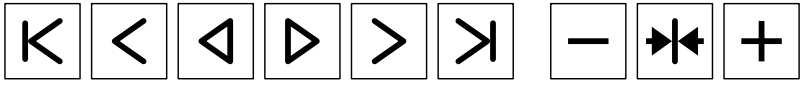




Bonus slide: Dynamic processes

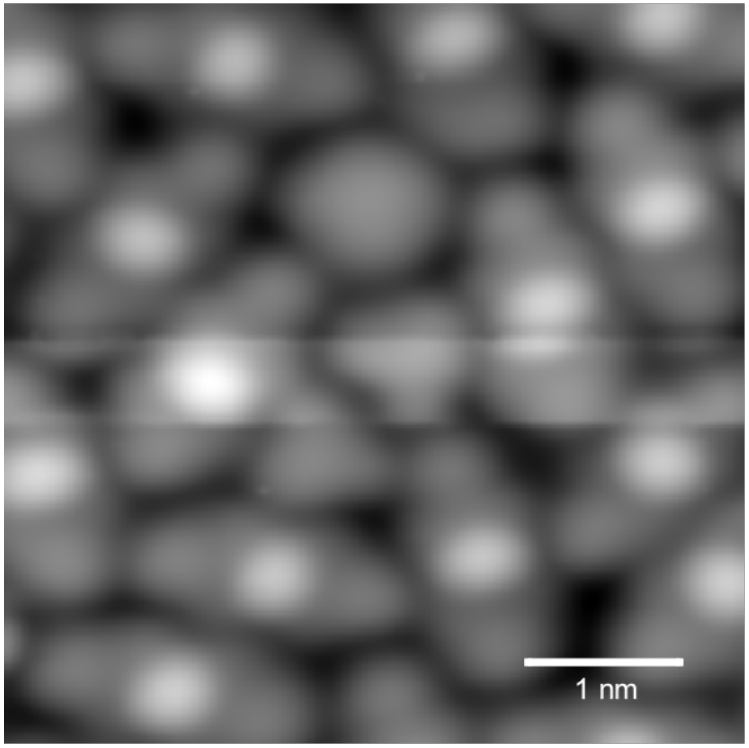
- Transitions between nanocavity modes

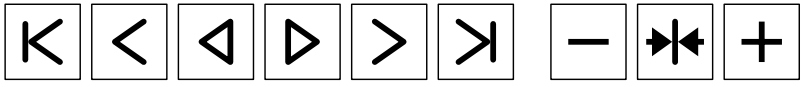




$7.8 \times 7.8\,\mathrm{nm}^2$, 200 mV, 60 pA

- Complex centre hopping
  - Common among $(\mathrm{NHC})_2\mathrm{Au}$ complexes





$4.8 \times 4.8\,\mathrm{nm}^2$, 100 mV, 50 pA