Assembling molecular templates

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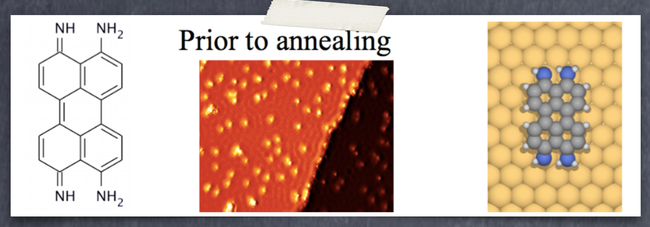
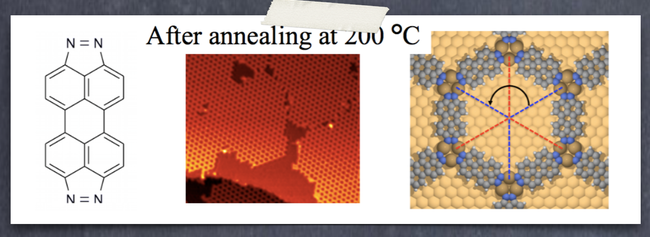
A bed worthy of nobility

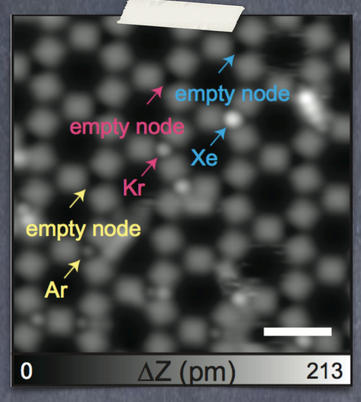


- Deposit DPDI (4,9-diaminoperylene-quinone-3,10-diimine) molecules onto Cu (111) surface).

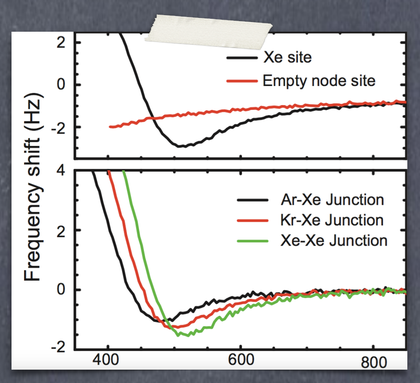


- Offers reactive nodes at junction of molecules due to copper-nitrogen complex.

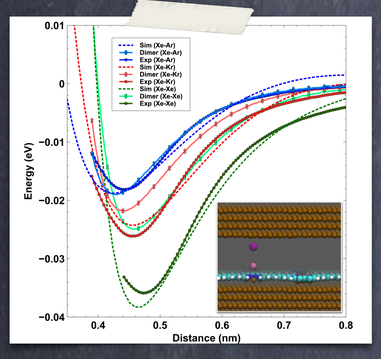
This one is weak in the force



- AFM tip can be controllably terminated with a Xe atom (Kr/Ar too difficult).
- Deposit noble atoms to DPDI, trapping them at nodes, then attempt to measure the direct "dimer" interaction - vdW.
- Measure frequency shift repeatedly over three characteristic noble atoms and get average curves.
- Subtract the empty site curve, to get the bare dimer interaction...in principle.

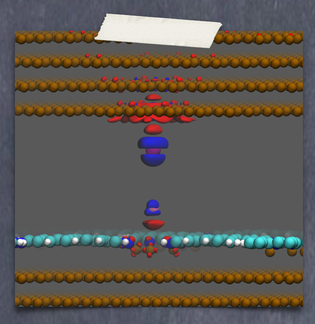


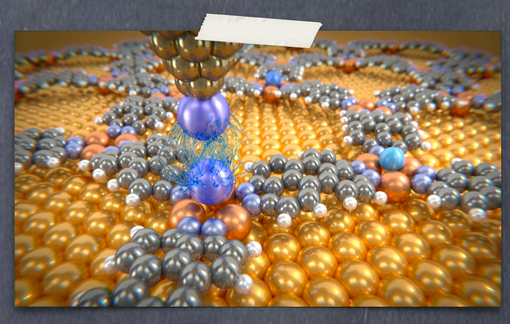
The nature of an atom...



- Subtle differences in the electronic structure at key distances, we see between full and empty sites - charge transfer and displacements.
- Despite the changes being tiny, they are deviations from atom-like behaviour - van der Waals dominates, but it is not purely "classical".

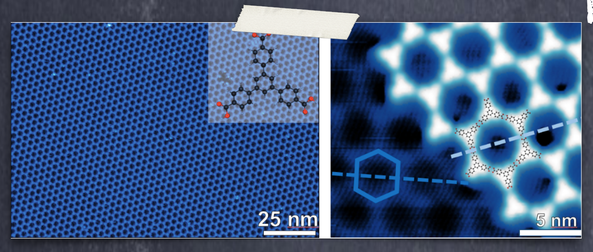
...and the colour of attraction



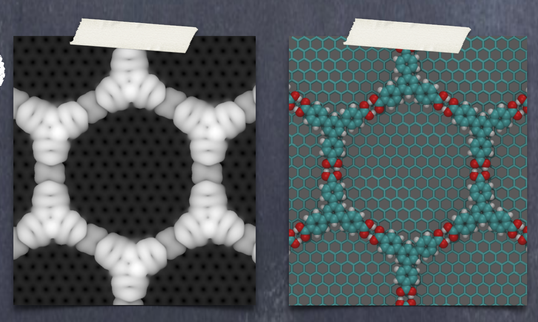


Nat. Commun. 7 (2016) 11559

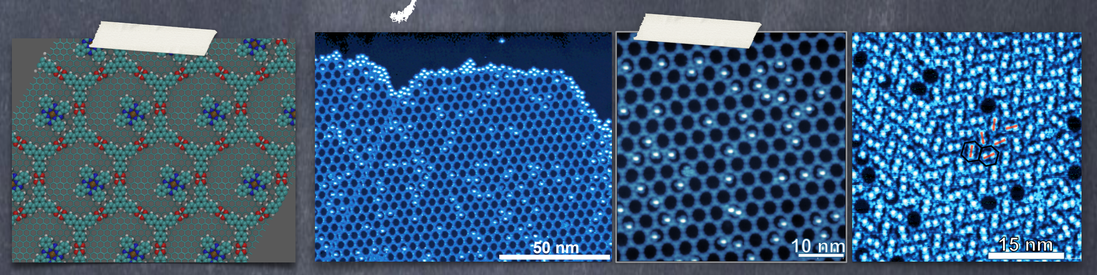
A molecular prison



- Deposit BTB (1,3,5-tris(4-carboxyphenyl)benzene) molecules onto graphene (Gr/Ir(111)).
- DFT predicts a stably H-bonded network.

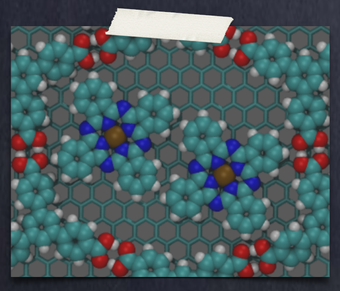


Solitary recommended

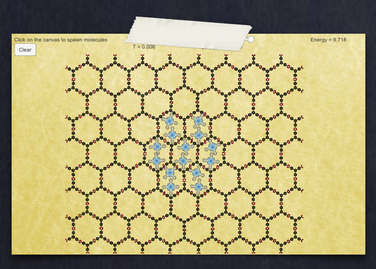


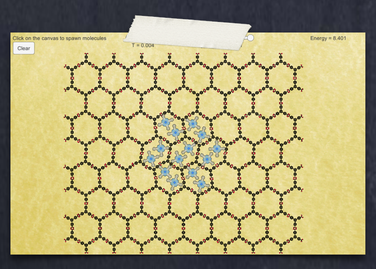
- Calculations show a clear preference for CoPC to bond at the edge of a pore, maximising O-H interactions.
- Adding a second CoPC causes a lot of distortion and is energetically unfavourable.

Better cell walls perhaps

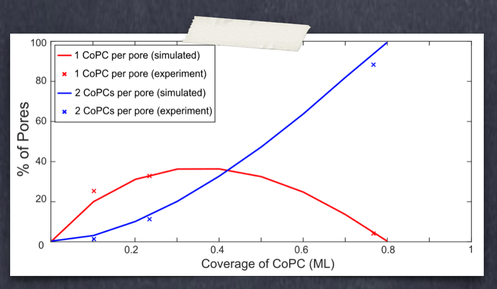


- Recalculate adsorption with average experimental pore distortion - now we can fit two molecules into a pore with comparable energy.



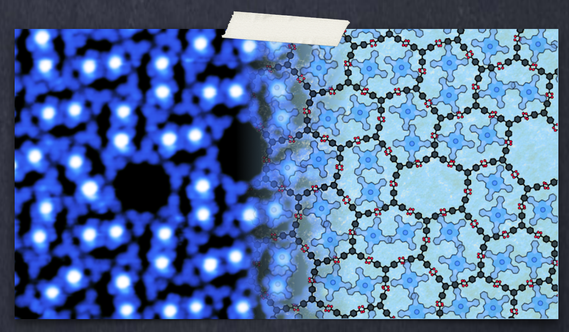


- Simple model based on elastic energy predicts distorted pores.



- Varying the dose and template provides control on nature of molecular lattice formed...
- Crossover from monomer to dimer matches.

Rehabilitation versus control



J. Phys. Chem. C 120 (2016) 8772

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