

Probing molecular interactions with NC-AFM and DFT

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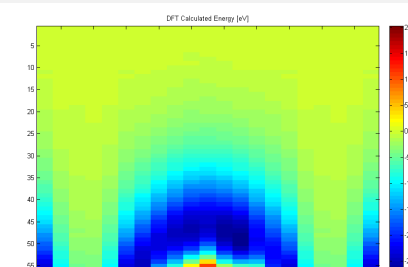
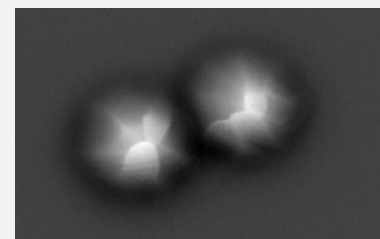
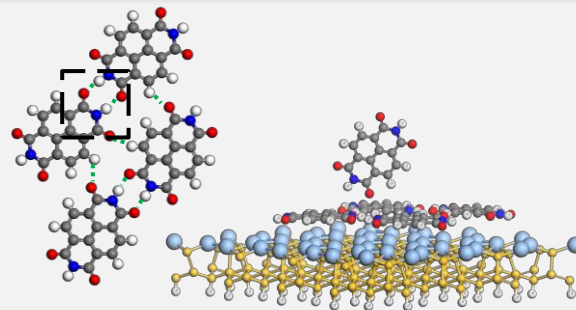
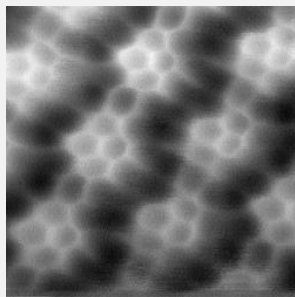
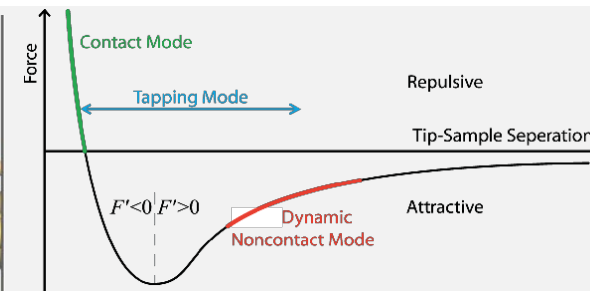
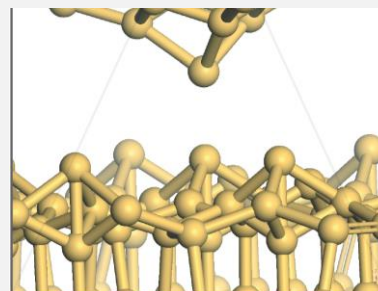


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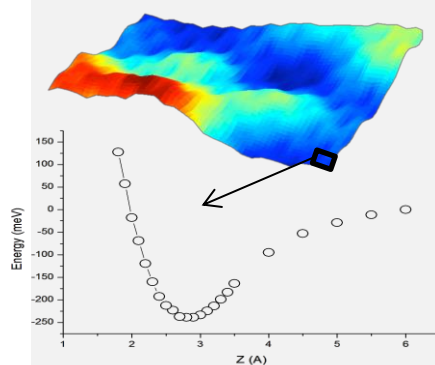
Non-contact atomic force microscopy.

- Experimental measurement of interatomic forces and energy potentials with atomic resolution.
- Used to measure the forces between molecules.
- Submolecular resolution imaging.



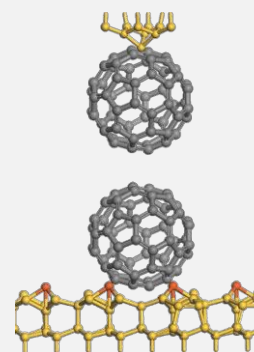
Intra & intermolecular imaging with NCAFM

- vdW-DFT used to calculate force spectra to investigate contrast formation.
- 30 x 30 x 11 (9,900) full DFT calculations required for simulated image



Molecular pair potentials.

- Calculate molecule-molecule interactions with vdW-DFT.
- Calculate grid of $F(z)$ to determine orientation dependence C_{60} interaction.



A.M.Sweetman, S. P.Jarvis, et al, Nature Comm., 5, 3931 (2014).

S. Jarvis, et al, J. Phys.: Condens. Matter, 27, 054004 (2015).

C. Chiutu, et al, Phys. Rev. Lett., 108, 268302 (2012).

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