Probing molecular interactions with NC-AFM and DFT

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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 C₆₀ interaction.