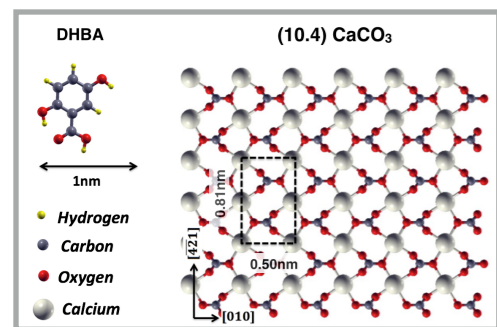


Temperature-driven Molecular Phase Transition

on a bulk insulator surface

Chiara Paris

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Experiments (Prof. A. Kunhle)

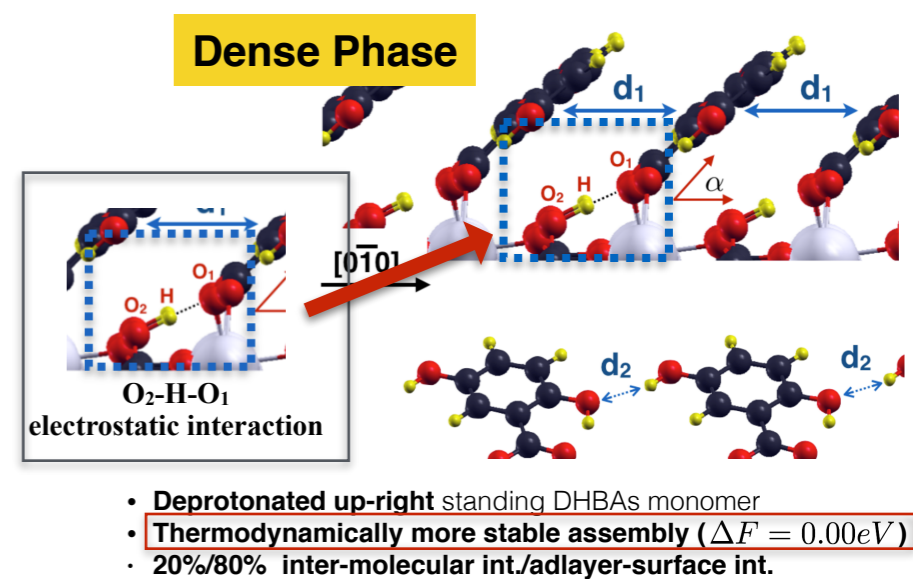
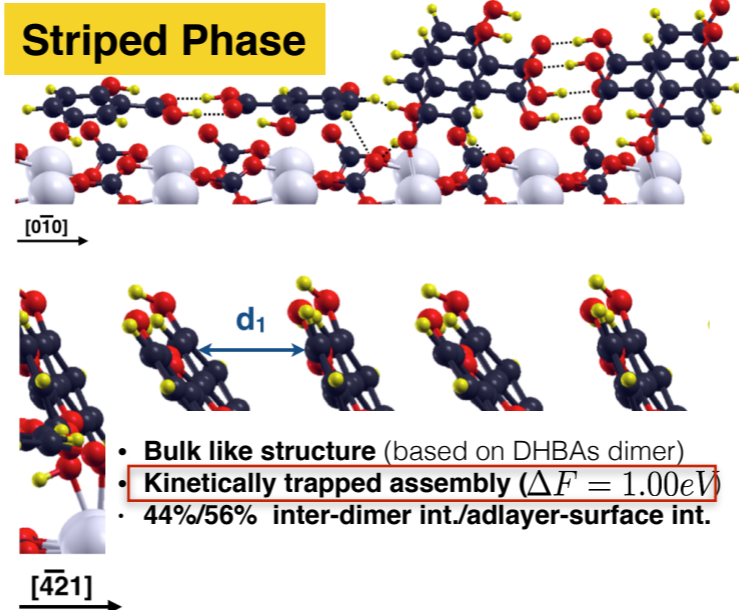
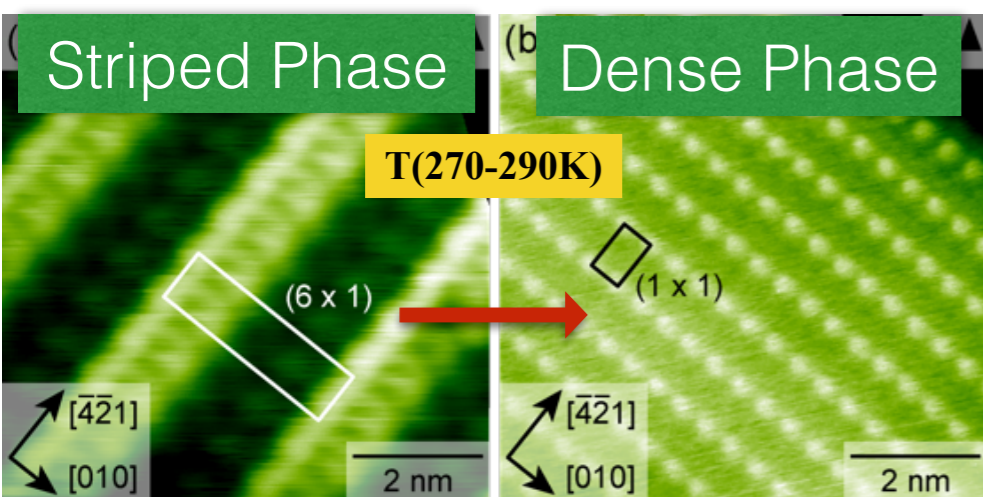
- Non-contact atomic force microscopy (NC-AFM)
- Kelvin probe force microscopy (KPFM)

Theory (Prof. L. Kantorovich)

Density Functional Theory (DFT) calculations

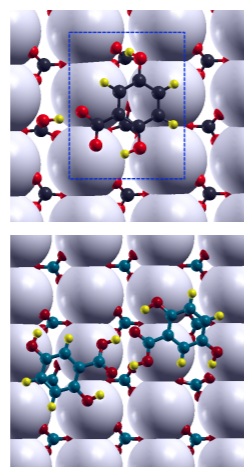
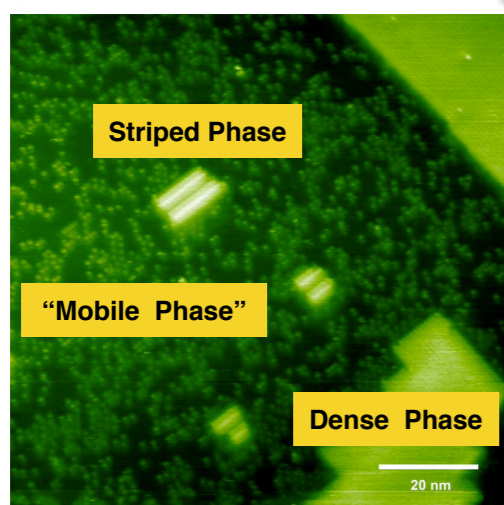
- Cp2k code
- Geometry relaxations, Mulliken charge analysis
- Energy Barriers via Nudged Elastic Band (NEB)

From the Striped to the Dense phase : Structural characterisation



Freezing the surface

Transition Mechanism: energy barriers via NEB calculations

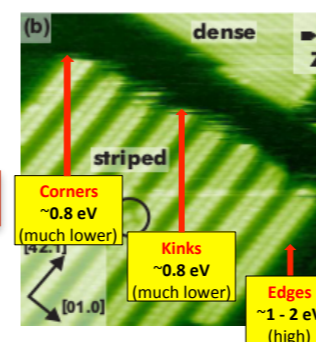


- DHBAs molecule and dimer adsorb on the surface**
- Diffusion barriers ($\sim 0.7eV$) \checkmark
 - Deprotonation (barrier-less) \checkmark
 - Protonation ($\sim 0.20eV$) \checkmark
 - Dimer formation (barrier-less) \checkmark
 - Dimer dissociation ($\sim 0.84eV$) \times

Striped phase forms first

Striped phase decomposition

Detachment barriers



- Molecule/dimer diffusion \checkmark
- Dimer dissociation \checkmark

Dense phase formation

Attachment barriers

