

## **Dynamical In Situ Microscopy: Using Theory to Fill in The Gaps**

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I shall review the limits on reaction rates that can be studied by dynamic in-situ TEM from a signal/noise perspective and from a consideration of reactant fluxes at gas pressures typical for these experiments. It will be shown that we are in a position to observe the deposition of single atomic layers per frame. Dynamic atomic resolution images give important clues on the way a reaction proceeds, but they don't tell the whole story. From the point of view of a single molecule arriving at the surface we still only observe the state of the system before and after the interaction. Density functional theory can play an important role in filling in the gap by calculating the energies along various possible reaction paths. Using plane wave pseudopotential based codes such as VASP or CASTEP it is possible to realistically calculate total energies for systems with up to 100 atoms, sufficient to model a gas molecule interacting with a surface. The activation energies can be used to derive rate constants that can be checked against growth rate measurements.

I shall illustrate some of these ideas with our work on carbon nanotube formation in the ETEM and how our calculations (and others) have effectively ruled out the hypothesis that carbon for nanotube formation is dissolved in the Ni catalyst particles.