Role of Adsorption in Growth of Nuclei and New Particle Formation

Objective: Investigate the adsorption hypothesis of Wang and Wexler using a density functional theory quantum mechanics

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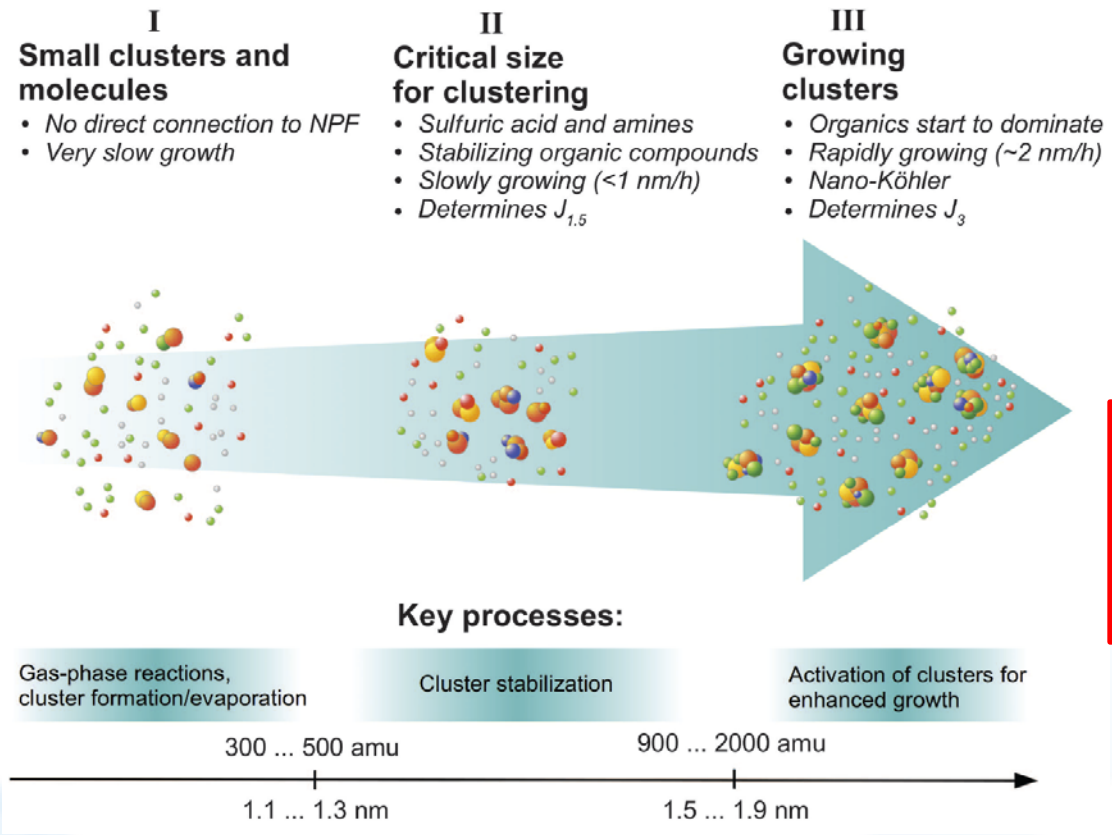
Collaborators: Jian Wang, Anthony Wexler

Funding status: NSF, DOE/BES, EMSL

Summary of progress: Cluster simulations performed and in progress to estimate adsorption ΔG and saturation ratio.

New particle formation- a two-step process



Kulmala et al., 2013

New particle formation: a two-step process:

- 1st step: sulfuric acid and amines, ammonia, or organic vapor form stable clusters
- 2nd step: organic vapor leads to enhance growth rate of the clusters to larger sizes.

Adsorption of organic molecules on the surface of nucleated clusters

Equilibrium *S* over growing particles:

$$S = \frac{C_\infty}{C_{Sat}} = \underbrace{\frac{\left[c-\theta\left(c-2\right)\right]-\sqrt{c^2\left(\theta-1\right)^2+4\theta c}}{2\theta\left(1-c\right)}}_{\text{Adsorption}} \cdot \underbrace{\exp\left(\frac{4v\sigma}{RTD}\right)}_{\text{Kelvin effect}}$$

$$\text{where } c = \exp\left(-\frac{\Delta G}{RT}\right)$$

S: Saturation ratio of organic vapor (i.e., C_∞/C_{Sat})

θ: Thickness of adsorbed organic molecules in layers (e.g. θ=1 for a monolayer)

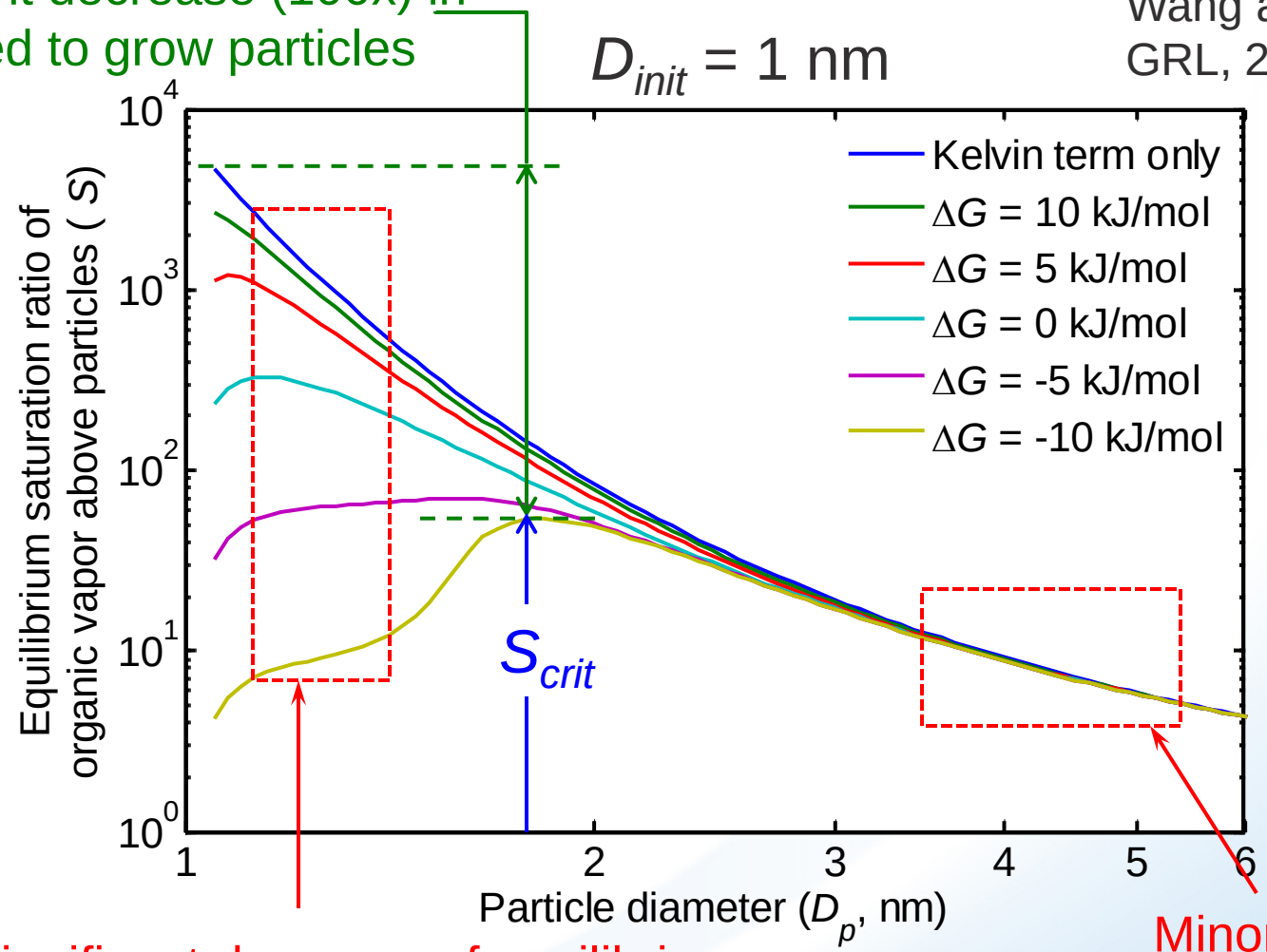
ΔG: The adsorption free energy for an organic molecule on the surface minus the free energy of adsorption on organic multilayer (i.e., liquefaction)

Wang and Wexler 2013 GRL

Effect of adsorption on equilibrium *S*

Significant decrease (100x) in *S* required to grow particles

Wang and Wexler, GRL, 2013



Significant decrease of equilibrium *S* during initial growth

Minor impact on later growth