

**TITLE**

**AUTHORS**

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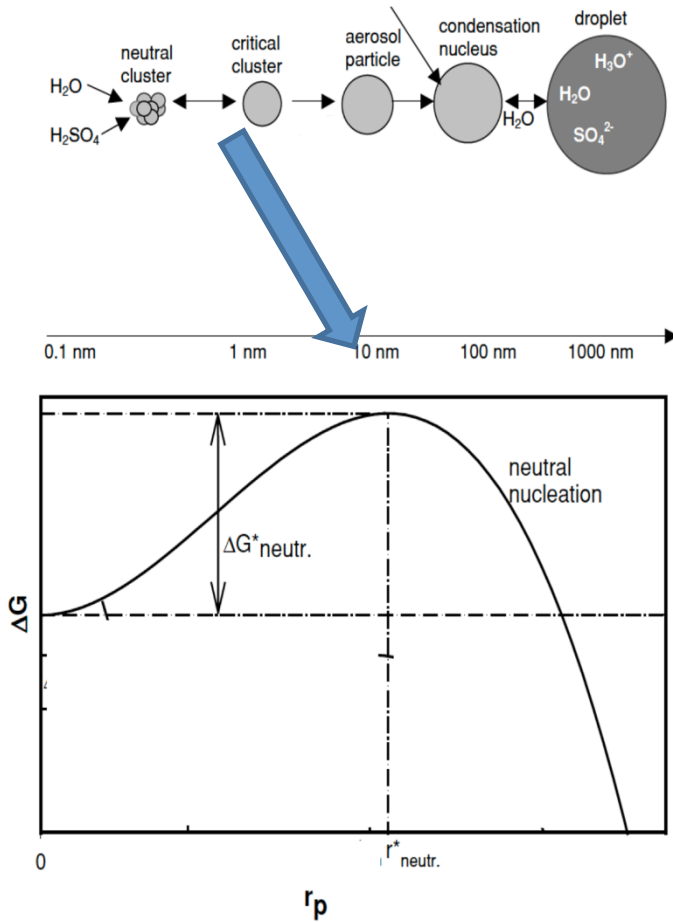


Figure 1: Aerosol formation and free energy of an aerosol system.

## Methodology

GAFF FF (T=80-250 K), TIP4P water, 10 ns MD simulation

50-300 sample configurations

B2PLYP/def-svp

Ri-MP2/aV[DTQ]Z extrapolation

thermodynamic corrections using B2PLYP/def-svp

Figure 2: A methodology combining classical molecular dynamics sampling with ab initio quantum mechanics methods.