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Growth of atmospheric freshly nucleated particles: a semi-empirical molecular dynamics study

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S1 Refined Single Point Energies

To obtain a general estimate of the interaction strength as a function of center-of-mass distance, we calculated the potential of mean force between $(SA)_{10}(AM)_{10}$ and SA through umbrella sampling (Torrie and Valleau, 1977) using the OPLS all-atom force field (Jorgensen et al., 1996). The umbrella sampling simulations were performed in LAMMPS (Large-scale Atomic/-
5 Molecular Massively Parallel Simulator (Plimpton, 1995; Thompson et al., 2022)) using the PLUMED plug-in (Tribello et al., 2014). We sampled center-of-mass distances from 6.0 to 40.0 Å in windows of 0.4 Å.

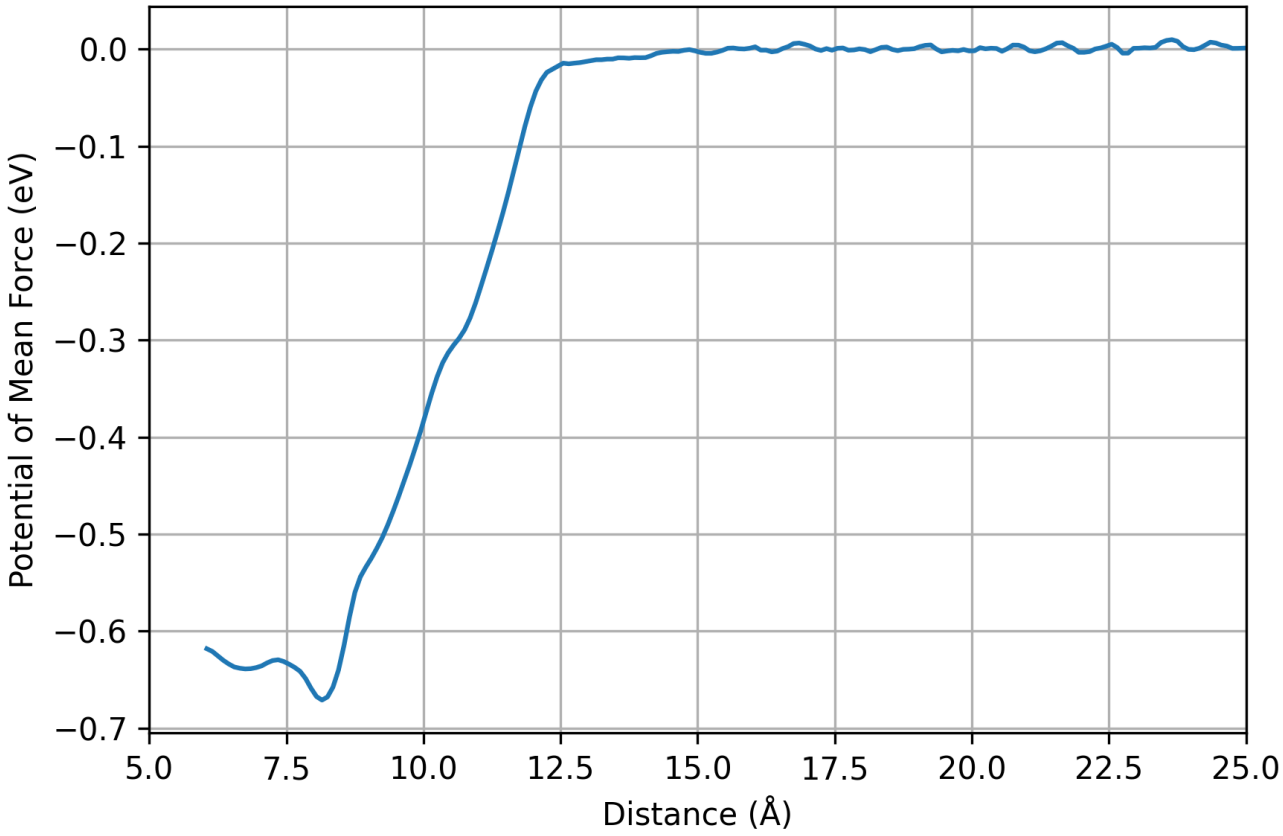

Figure S1. The potential of mean force for the $(SA)_{10}(AM)_{10}$–SA system using OPLS-all atom force field.

In each window, the $(SA)_{10}(AM)_{10}$–SA system was placed at the corresponding distance and equilibrated for 1 ns using a Langevin thermostat (Schneider and Stoll, 1978; Bussi and Parrinello, 2007) at 300 K with a bias potential of 4 eV/Å, followed saby a 100 ns production run employing a canonical sampling through velocity rescaling thermostat (Bussi et al., 2007) and a
10 bias potential of 0.5 eV/Å. The timestep of the simulations was set to 1 fs. Following the simulations, the free energy profile was constructed using the WHAM code (Grossfield, 2002). The PMF was then corrected by adding the term $+k_{\mathrm{B}}T\ln r^2$ to account for configurational entropy. Force field parameters for OPLS were taken from Loukonen et al. (2010).

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