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Energetic analysis of succinic acid in water droplets: insight into the size-dependent solubility of atmospheric nanoparticles

Chuchu Chen[1,2], Xiaoxiang Wang[1,6], Kurt Binder[3], Mohammad Mehdi Ghahremanpour[4,5], David van der Spoel[4], Ulrich Pöschl[2], Hang Su[2], and Yafang Cheng[1]

[1]Max Planck Institute for Chemistry, Minerva Research Group, Germany (c.chen@mpic.de)
[2]Max Planck Institute for Chemistry, Multiphase Chemistry, Mainz, Germany
[3]Johannes Gutenberg University of Mainz, Institute of Physics, Mainz, Germany
[4]Uppsala University, Department of Cell and Molecular Biology, Uppsala, Sweden
[5]Yale University, Department of Chemistry, New Haven, USA
[6]Southern University of Science and Technology, School of Environmental Science and Engineering, Shenzhen, China

Size-dependent solubility is prevalent in atmospheric nanoparticles, but a molecular level understanding is still insufficient, especially for organic compounds. Here, we performed molecular dynamics simulations to investigate the size dependence of succinic acid solvation on the scale of ~1-4 nm with the potential of mean forces method. Our analyses reveal that the surface preference of succinic acid is stronger for a droplet than the slab of the same size, and the surface propensity is enhanced due to the curvature effect as the droplet becomes smaller. Energetic analyses show that such surface preference is primarily an enthalpic effect in both systems, while the entropic effect further enhances the surface propensity in droplets. On the other hand, with decreasing droplet size, the solubility of succinic acid in the internal bulk volume may decrease, imposing an opposite effect on the size dependence of solubility as compared with the enhanced surface propensity. Meanwhile, structural analyses, however, show that the surface to internal bulk volume ratio increases drastically, especially when considering the surface in respect to succinic acid, e.g., for droplet with radius of 1 nm, the internal bulk volume would be already close to zero for the succinic acid molecule.