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Comment on acp-2020-1329

Anonymous Referee #1

Referee comment on "Energetic analysis of succinic acid in water droplets: insight into the size-dependent solubility of atmospheric nanoparticles" by Chuchu Chen et al., Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2020-1329-RC1, 2021

The solvation of succinic acid has been investigated in this interesting piece of work. The simulations were conducted for a single succinic acid molecule for different sizes of water nanodroplets (i.e., droplet 255 radius from ~1 nm to 4 nm) and different thickness of water planar slabs (i.e., half slab thickness from ~1 nm to 4 nm). These simulations reveal a stronger surface propensity for succinic acid to stay on the surface of a curved surface rather than on a planar one, due to changes on the hydration energetics associated with the curvature of the nanodroplets.

This is an interesting finding that may have impact for the description of the chemistry of nanodroplets and maybe atmospheric aerosols, even if the later link is not fully established in this work.

It has been shown in previous studies that indeed there is an energy minimum at the air/water interface, which may indeed lead to isolated molecule to have a propensity to stay on the surface. Is this study another simple highlight of the compound dependent feature or is there a benefit of the present work? Maybe the authors could strengthen their message to underline better their key findings (such as the size dependence)? (Note that a revision of the use of the English language would also help, as a several sentences are difficult to follow).

Obviously, one key finding can be found in the observed size and shape dependence. However, the simulations were made on very small objects with limited amount of water, where one can wonder if the difference between bulk and surface is real (especially when the surface region is mentioned to be one nm thick). This is certainly an obvious comment that the authors could address easily for the wider audience of ACP.

While the choice of succinic acid is relevant to the atmosphere, this diacid certainly require

an extra amount of water for full solvation. In a context of a limited amount of water (fixed by definition on these simulations), this reviewer was wondering if this would also affect the observations made here where this molecule was pushed to the surface?

Finally, to get closer to atmospheric applications is there any indication for which droplet size this “surface push” is applicable.