



EGUsphere, referee comment RC2
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Comment on egusphere-2022-826

Anonymous Referee #2

Referee comment on "Microphysics of liquid water in sub-10 μ m ultrafine aerosol particles" by Xiaohan Li and Ian C. Bourg, EGU sphere,
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The authors present a theoretical study of nanoparticle morphology and gas/droplet partitioning behavior of water using systems consisting of sodium chloride, water, and pimelic acid. The authors discover several parameters - sphericity and fractional surface coverage - that aptly describe chemical morphology as a function of composition and size regimes and variation in mass accommodation coefficients. The authors also report a threshold for the validity of continuum theories. The paper is well-written and is of interest to the Atmospheric Chemistry and Physics community, and is recommended for publication after the following general comments have been addressed.

As the authors note in Section 3.4, classical water models are known to have biases in errors in reproducing experimental surface tensions - though with SPC/E having one of the smallest errors (Vega and de Miguel, 2007). Additionally, a study (Lbadaoui-Darvas and Takahama, 2019) suggest that carboxylic acid-water dynamics are not well captured in equilibrium MD simulations and lead to deviations in predictions of water activity even above 0.95. On the other hand, the water activity calculations seem to suggest that the simulation results are in good agreement - with observations - is this due to canceling of errors (e.g., with molar volume) or the relatively small magnitude of the error in surface tension by these models?

Many of the conclusions summarize the effect of "organic loadings" but the simulations use a specific type of organic, namely pimelic acid. Many studies on the other hand suggest the importance of alcohols in marine aerosols (e.g., Russell et al., 2010). Is there reason that the authors can justify broadening the conclusion from a particular "organic acid" to "organics" generally? Other abundant dicarboxylic acids (e.g., oxalic acid) may also exhibit different bulk/surface partitioning behavior than demarcated by the sphericity factor. The main question is whether parts of the manuscript should be more clear in what is meant by "organic loading" in this work.

References:

Lbadaoui-Darvas, Mária, and Satoshi Takahama. "Water Activity from Equilibrium Molecular Dynamics Simulations and Kirkwood-Buff Theory." *The Journal of Physical Chemistry B* 123, no. 50 (December 19, 2019): 10757–68. <https://doi.org/10.1021/acs.jpcc.9b06735>.

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Vega, C., and E. de Miguel. "Surface Tension of the Most Popular Models of Water by Using the Test-Area Simulation Method." *The Journal of Chemical Physics* 126, no. 15 (2007): 154707. <https://doi.org/10.1063/1.2715577>.