

STABLE DROPLETS AND BUBBLES WITHIN THE FUNDAMENTAL MEASURE DFT

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It was predicted [1] that condensation in the Earth's atmosphere occurs at very low vapor supersaturations due to the presence of submicron hydrophilic aerosols, on which stable and critical droplets can form. Recently, with the use of the squared-gradient density functional theory (DFT), we found [2,3] stable droplets and bubbles around solid lyophilic and, respectively, lyophobic particles. Such droplets and bubbles corresponded to the local minima of the system grand potential. This work aims to validate these results within more rigorous fundamental measure DFT [4].

The density profiles in the fluid around spherical particles with different particle-fluid interaction parameters were computed through numerical minimization of the grand potential using classicalDFT library [5]. Stable droplets as liquid films around lyophilic particle in vapor are observed if the fluid chemical potential is less than certain threshold value. Stable bubbles (vapor shells) form around lyophobic particle in liquid if the fluid chemical potential is larger than another threshold value. If the thresholds are reached, the stable and critical new phase nuclei coincide. New results demonstrate visible structural layering in the density profiles in comparison with the squared-gradient DFT profiles [2,3], but are in fair agreement with them.

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References

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