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Density Functional Approach to Investigate the Stability of Nanobubbles GOTA KIKUGAWA, SHU TAKAGI, YOICHIRO MATSUMOTO, The University of Tokyo — Recently, some experimental results showing the existence of nanobubbles which are bubbles of tens or hundreds of nanometer diameter in water have been reported. However, it is generally considered that such tiny bubbles are inherentlyunstable because of a strong effect of surface tension. Therefore, the stability of the nanobubbles are regarded as an unresolved problem. In order to investigate the stability mechanism, our approach is based on a microscopic standpoint. Especially, we introduced the density functional theory of classical systems to take into account the microscopic information on gas– liquid interface and to execute the stability analyses in the microscopic system. The density functional approach has many advantages in the stability analysis of the two-phase microscopic system compared with the molecular dynamics approach. First, natural external conditions such as the grand canonical ensemble can be imposed. Second, the free energy evaluation which is required in the stability analyses can be performed directly. In this study, we focused on the effect of impurities in water on the stability of the nanobubbles. In the experimental system, electrolytes or surfactants are usually used in the literature, and we consider that the effect of the impurities is crucial.

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