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**Theoretical simulations of non-contact atomic force microscopy in aqueous environment** MASANORI HARADA, MASARU TSUKADA, Waseda University — Most of the theoretical simulations of atomic force microscopy (AFM) use the models consisting of only the tip and sample and have been in qualitative agreement with the experimental images especially of inorganic surfaces in vacuum. However, such models are not suitable for the AFM experiments performed in liquid. One methodology to improve the models is to incorporate the liquid molecules into the models as they exist in experimental environments. However, the methodology needs more enormous computational costs because of the increase of atom number and the increase of the time scale of simulations in order to reproduce the equilibrium property of the liquid. To overcome this difficulty, Koga et al. used statistical method called RISM for contact mode AFM simulations using the artificial model of tip and sample [1]. We use the similar methodology for nc-AFM simulations of more realistic models of tip and sample. [1] K. Koga et al., Phys. Rev. B 60, 14328 (1999).

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