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氏名／専攻・学年 Name / Department	Hari Krishna Chilukoti/ Nanomechanics
学会名 Conference's name	The 12th International Symposium on Fluid Control, Measurement and Visualization (FLUCOME 2013)
開催地 Venue (Name of the facility, city & country)	Nara Prefecture New Public Hall, Nara, Japan
日程 Conference period	November 19-23, 2013
発表タイトル Presentation Title	Study of alkane chain length influence on structure and dynamic properties at intrinsic liquid-vapor interfaces

【発表概要　Brief summary of your presentation】

Molecular level understanding of structure at interfaces has applications in engineering and biological process. In the present study, molecular dynamic simulations were used to study the intrinsic structure at liquid-vapor interfaces of alkanes. Local and instantaneous interface definition proposed by Kikugawa et al. was used in the present study. Density profiles and order parameters were calculated with respect to the distance from the intrinsic interface for decane and tetracosane. The layering structure of alkane molecules at the liquid-vapor interface was observed as the pinned structure of alkane liquids based on the intrinsic surface. Decane and tetracosane density profiles have the same number of oscillations in the interface region at the considered temperatures. By examining the orientation order parameter, molecular ordering at the interfaces was observed. It was found that liquid molecules are preferentially oriented more parallel to the intrinsic surface when comparing with the ordering property which is evaluated as a function of distance from the Gibbs dividing surface at a particular temperature for decane and tetracosane.it was found that self-diffusion coefficient parallel to the intrinsic interface varied steeply than the values obtained with respect to the Gibbs dividing surface.

【他の講演等から得られた知見、感想等。What you learned from other presentations, general impression you had, etc.】

An atomistic molecular dynamics simulation of hydronium ions and water molecules transport in the nanostructure of hydrated Nafion membrane is studied by systematically changing the hydration level. The new empirical valence bond (EVB) model is developed based on the previous study of EVB model to improve description of proton mobility in both aqueous and Nafion environments. They have calculated mean square displacement (MSD) to determine diffusion coefficients of hydronium ions and water molecules as a function of hydration level for the investigation of the impact of Grotthuss mechanism on the transport property of solvent molecules as well as the validation of our simulation by comparing with the experimental data of diffusion coefficients. A large contribution of Grotthuss mechanism for the diffusion of hydronium ions has been found and this implies the important fact of Grotthuss mechanism in the membrane as well as in the bulk aqueous solutions.

They have evaluated liquid-vapor coexistence curve for quintet oxygen using an *ab-initio* intermolecular potential function. The intermolecular potential for quintet oxygen was based on the molecular orbital (MO) calculations performed by Bartolomei et al. and expressed by spherical harmonics expansion. The result showed good agreement with experimental data except around the critical point although oxygen has other spin multiplicity states; singlet and triplet. Besides, this potential is just two-body intermolecular potential and does not include many-body effect. So, the potential function for quintet oxygen does not consider many physical elements (triplet, singlet, and many-body effect) and it is possible that the result shows good agreement by ignoring both spin multiplicity and many-body effect. Next, they compared the potential energy surfaces (PES) for the quintet, triplet, and singlet spin multiplicity. The result showed that these PESs quantitatively differ especially in the equilibrium distances and the well depths at several geometries. Therefore, these results suggest that the effect of the triplet and the singlet multiplicities is not negligible for the thermophysical properties against the quintet multiplicity.

The aerostatic bearing has been researched and developed as being the most important machine element of the ultra-precision machine, and stable performance has finally been obtained. To expand the scope of application by exploring the characteristics of the air bearing, applications to the small-diameter, ultra-high speed spindle as well as development of the ultra-high speed aerostatic bearing spindle, which is driven by an air turbine, has been pursued. Methods of evaluating precision and stiffness of the aerostatic bearing spindle have been estimated. However, there is no method of evaluating power output performance. Therefore, we have studied the method of quantifying the power output by using, as a load, a windage (air friction) loss resulting from the rotation of a disc mounted to the ultra-high speed spindle end.