Analysis of molecular energy transfer for the design of thermal medium fluids

T. Ohara[1], H. Matsubara[1], and G. Kikugawa[1]

[1] *Institute of Fluid Science, 980-8577, Sendai, Japan*

Molecular dynamics simulation is gaining sufficient performance for research of thermophysical properties, especially transport properties, of fluids and soft matters in these days. It works not only to predict values of thermophysical properties even at any extreme conditions, but also to elucidate the fundamental mechanisms that determine the thermophysical properties. These are two key functions of the engineering research field of "molecular thermophysical properties".

Here we present a part of our systematic study on thermal conductivity of some typical fluids. To "analyze" thermal conductivity, an approach of the decomposition of heat flux [1–3] was applied and molecular origin of thermal energy transfer between and in the molecules was examined. Thus, the contributions of functional groups in a molecule to the thermal energy transfer were isolated and each contribution was evaluated quantitatively.

To characterize the functions of each group, a concept of the atomistic heat path (AHP) [4–7] has been proposed. The thermal energy transfer in each molecule and between each pair of molecules resulting from each force, i.e., van der Waals force, Coulomb force or the force due to covalent bond, is assumed as an AHP. The total thermal energy transfer by a kind of AHP, which constitutes thermal conductivity and is called as partial thermal conductivity, is given by the product of number density of AHPs in the space and efficiency of thermal energy transfer per an AHP. Characteristics of two factors of AHP are presented.

[1] T. Ohara, J. Chem. Phys., 111 (1999), 6492. [2] D. Torii et al., J. Chem. Phys., 128 (2008), 044504. [3] T. Ohara et al., J. Chem. Phys., 135 (2011), 034507. [4] H. Matsubara et al., J. Chem. Phys., 142 (2015), 164509. [5] Y.-P. Fang et al., Fluid Phase Equilibria, 429 (2016), 293. [6] H. Matsubara et al., Int. J. Heat Mass Transfer, 108 (2017), 749. [7] H. Matsubara et al., Fluid Phase Equilibria, 441 (2017), 24.

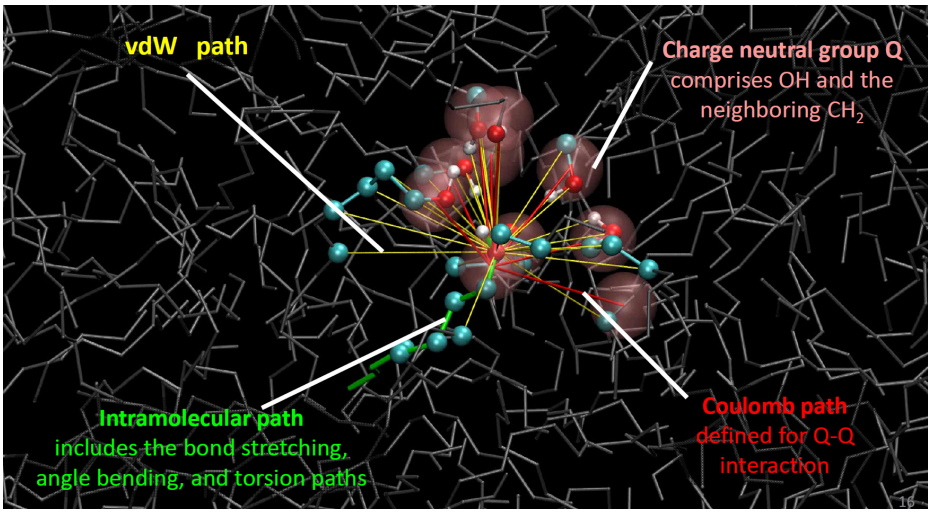

Fig.1 Atomistic heat path in liquid octanol