第410回触媒科学研究所コロキウム

Molecular modeling of ice–air and water–air interfaces: input from theoretical sum–frequency generation spectroscopy

Dr. Yuki Nagata

(Max Planck Institute for Polymer Research, Mainz, Germany)

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When water is in contact with air phase, the water hydrogen-bonded network is interrupted, differentiating the properties of interfacial water from that of bulk water. I shall focus on the water–air interface [1] and ice–air interface [2] and aim at revealing the anomaly of the water at these interfaces through theoretical sum–frequency generation technique. Furthermore, I would like to discuss how water can evaporate at the water–air interface. [3]

[1] F. Perakis, L. De Marco, A. Shalit, F. Tang, Z.R. Kann, T.D. Kühne, R. Torre, M. Bonn, Y. Nagata, Chem. Rev. 116, 7590 (2016) [2] W. Smits, F. Tang, M. A. Sánchez, E. H. G. Backus, L. Xu, T. Hasegawa, M. Bonn, H. J. Bakker, Y. Nagata, Phys. Rev. Lett., 119, 133003 (2017) [3] Y. Nagata, K Usui, M Bonn, Phys. Rev. Lett., 115, 236102 (2015).

Yuki Nagata studied chemical system engineering at the University of Tokyo in Japan and obtained his bachelor (2002) and master (2004) degrees. He then joined the group of Prof. Yoshikata Tanimura at the Kyoto University also in Japan for a PhD project and earned his PhD degree in 2007. From 2007 to 2009 he worked as a research scientist at BASF SE in Germany. From 2009 to 2011 he worked at the University of California, Irvine, US, with Prof. Shaul Mukamel as a PostDoc. Since August 2011 he has been working at the Max Planck Institute for Polymer Research as a Group Leader (Director: Prof. Mischa Bonn). His research focus is on the structure and dynamics of water at the lipid/air/solid interfaces by using theoretical/computational approaches.

問合せ先：触媒科学研究所　中山哲（nakayama@cat.hokudai.ac.jp 011-706-914）