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Structure of Imidazolium-based Ionic Liquids MARIE-LOUISE SABOUNGI, IMPMC, Université Pierre et Marie Curie, CNRS-UMR 7590, 75005 Paris and Universite d'Orleans, Orleans, France, MIGUEL GONZÁLEZ, Institut Laue Langevin, 6 rue Jules Horowitz, BP 156, 38042 Grenoble Cedex 9, France, BACHIR AOUN, Advanced Photon Source, Argonne National Laboratory, IL 60439, USA, OLEG BORODIN, Army Research Laboratory, Adelphi, MD 20783, USA, WESLEY HENDERSON, North Carolina State University, Raleigh, NC 27695-7905, USA, SHINJI KOHARA, JASRI, 1-1-1 Kouto, Sayo-cho, Sayo-gun, Hyogo 679-5198, Japan, MAIKO KOFU, OSAMU YAMAMURO, Institute for Solid State Physics, University of Tokyo, Chiba 277-8581, Japan — Room-temperature ionic liquids (RTILs) are receiving increased attention due to their unique properties, including nonvolatility and solvating capability, leading to a wide range of potential uses in catalysis, separation technology, photovoltaics, batteries and fuel cells. We have studied the structures of liquid and solid 1-ethyl, 1-butyl and 1-hexyl-3-methylimidazolium bromide with high-energy x-ray diffraction measurements and atomistic molecular dynamics numerical simulations. Excellent agreement between experiment and simulation is obtained, including the region of the low-Q peak that characterizes the nanoscale heterogeneity in these liquids. Significant changes in this heterogeneity are observed when water is added to the ionic liquid, depending on the length of the ethyl chain. With a longer (octyl) chain length, the degree of heterogeneity is enhanced, possibly reflecting the water nano-domains observed in simulations.

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