Nanotek-2013

OMICS Group Conferences
Accelerating Scientific Discovery

3rd International Conference on
Nanotek & Expo

December 2-4, 2013 Las Vegas, USA

Dynamics of protonic transport through the nanochannel water in molecular porous crystals

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Abstract

Confined water in nanometer-scale geometries has interdisciplinary importance because such water molecules hold unique properties like rapid flow rate and high proton conductivity relating to functionalities of biological materials, fuel cells, and applications for selective filters, nanofluidics devices, etc. Among wide variety of porous materials, single-file water molecules embedded in carbon nanotube are considered as a typical-model system for physicists, and many computer simulations have been performed so far. Nevertheless there is a little experimental result owing to the difficulty to obtain good single crystal. In high-quality molecular porous crystals with millimeter-order length, we have performed systematic studies on crystal structural analysis, infrared spectrum and microwave conductivity. In $\{[Co^{III}(H_2bim)_3(TMA)\ 20H_2O]_n$ salt, we have already reported that the water nanotube (WNT) embedded in the hydrophilic nanochannel is an intrinsic proton conductor with high mobility. The proton and protonic hole form Eigen-type hydrates, around which local distortions are induced. In $\{[Co^{III}(H_2bim)_3(TATC)\ 7H_2O]_n$ salt, we have obtained for the first time much narrower nanochannel accommodating the highly one-dimensional water chain constructed by 6 water molecules per unit. The proton and protonic hole forming Eigen-type hydrates also exist in the water chain, whereas the conducting property is huge different from one in WNT. We expect that the proton and protonic hole are respectively combined with D and L configurational defects, and these carriers transfer through the antiferroelectric-ordered water chain. The protonic transport and the ordering of water chain must be dominated by the interfacial interaction in connection with the charged site in the framework.

Biography

Hiroshi Matsui has earned his Ph.D in 1992 from Tohoku University, Japan. Afterwards, he became JPSJ research fellows (1992-1994) and experienced postdoctoral studies in Clarendon Laboratory, Oxford University (1994-1995). In 1995, he moved to Osaka Prefecture University, Japan. In 1998, he returned to Tohoku University, and now he is the associate professor. Hiroshi Matsui is an expert in optical properties of solids with extremely wide range of electromagnetic waves. He has published more than 100 papers in reputed journals. For his recent studies, he was awarded JPSJ papers of editors' choice in 2010.