Poster Presentation

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The structure of one-dimensional water nanowire at room temperature

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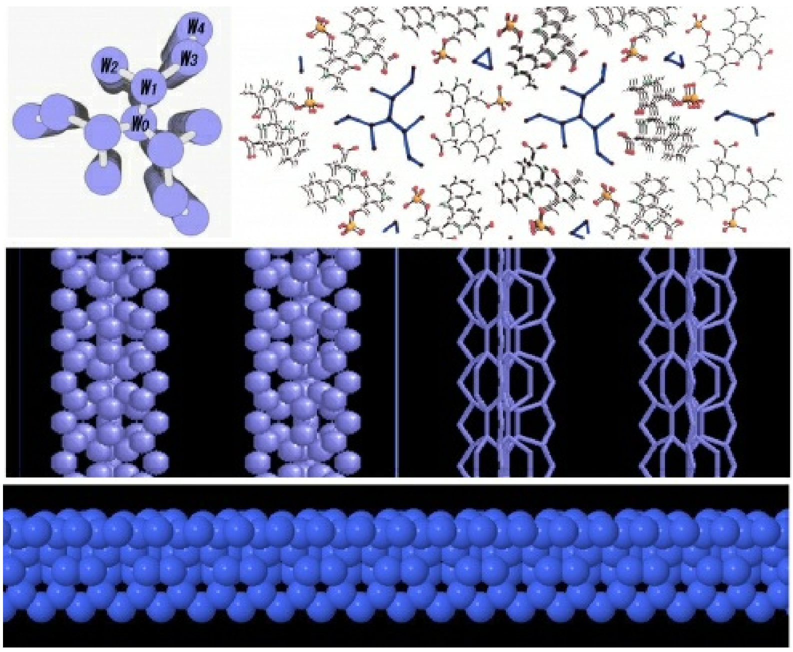
During the last decade large interest has been devoted to one-dimensional (1D) nanowires, and much experimental research has been directed towards making material nanowires. As far as the water molecule is concerned, its 3D solid state, i.e., ice has been widely studied and many structures have been already reported. In contrast, the information concerning the 1D water nanowire of diameter > 1 nm is quite lacking. Recently, we clarified a successive and columnar 1D water structure in the single crystal prepared by mixing the aqueous solution of L-tryptophan and pyridoxal-5-phosphate. This 1D water nanowire structure (diameter= 1.641 nm) is stable at room temperature (293 K) and best similar to the hexagonal ice (Ih), the naturally occurring ice in nature. Inner part of this nanowire is completely the same as ice Ih, where three boat-type hydrogen-bonded six-membered water rings are formed around a 3-fold symmetry axis. Moreover, it is noteworthy that this nanowire is constructed by piling up the double layers of mirror-image symmetry, and similar mirror-image arrangement of double layer is also formed in ice Ih. In the case of this nanowire, 26 water molecules form a water cluster unit consisting of mirror-image double layers, and the repeated distance of this nanowire is ca. 0.946 nm. This value equals to the double size of cell constant c, and is nearly equal to the double of the fundamental spacing of ice Ih, 0.474 nm. Outer side of this nanowire is alternatively arrayed by five- and seven-membered rings parallel to the 3-fold axis, and the outermost three-cornered portions of (-W3--W4-)n form infinite planar zigzag chain structures. The overall structure of this nanowire could be described as an infinite three-square column in nanospace, constructed by hydrogen-bonded water molecules. This column structure is formed in a channel constructed by piling up of circular cluster unit consisting of six organic host molecules. Previously, we obtained a similar hollow-type water nanowire (diameter= 1.649 nm) crystallized from heavy water reported in previous conference. However, this type of nanowire was unstable above 220 K, and two of five independent water molecules were lacked at 293 K.[1] In contrast, the present structure is stable at room temperature (293 K). Therefore, we believe that this 1D water nanowire structure presented here provides the structural scaffold for evaluating one-dimensional water science, such as the water transfer or the conduction of protonic current through pores across membrane.

[1] Wakahara, A. & In, Y. (2014) Acta Cryst. A70, C565.



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