Inclusion and dynamics of a polymer–Li salt complex in coordination nanochannels

Nobuhiro Yanai, Takashi Uemura, Satoshi Horike, Satoru Shimomura, and Susumu Kitagawa

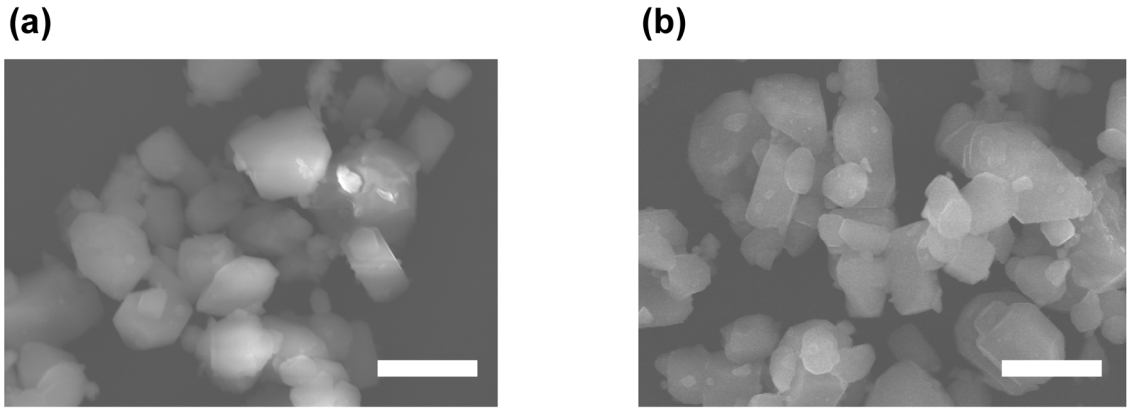

Fig. S1 SEM images of (a) **1** and (b) **1**⊃PEG(Li^+). Scale bars = 10 μm.

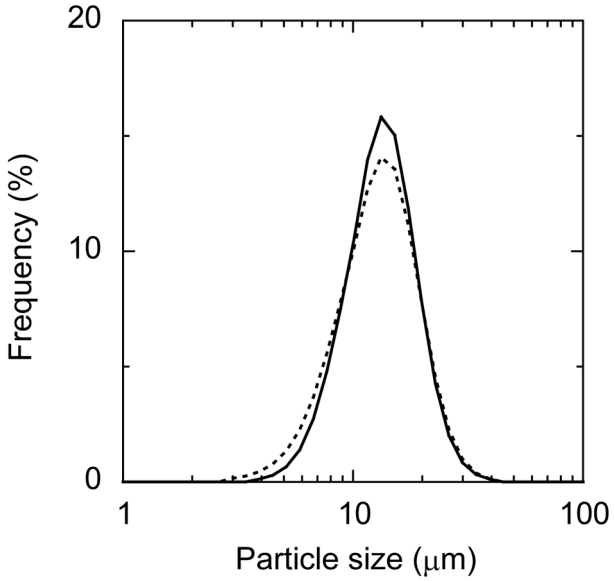

Fig. S2 Particle size distributions of **1** (dashed line) and **1**⊃PEG(Li^+) (solid line) evaluated by laser light diffraction.

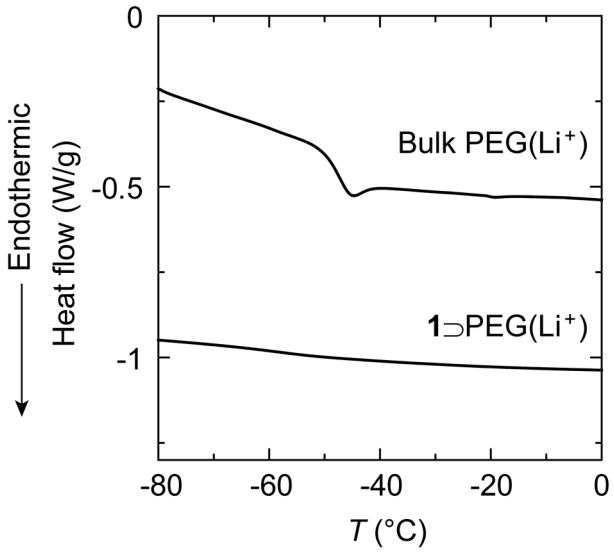

Fig. S3 DSC heating curves of bulk PEG(Li^+) and **1**⊃PEG(Li^+). The heating rate of the measurements was 10 K min^{-1}.

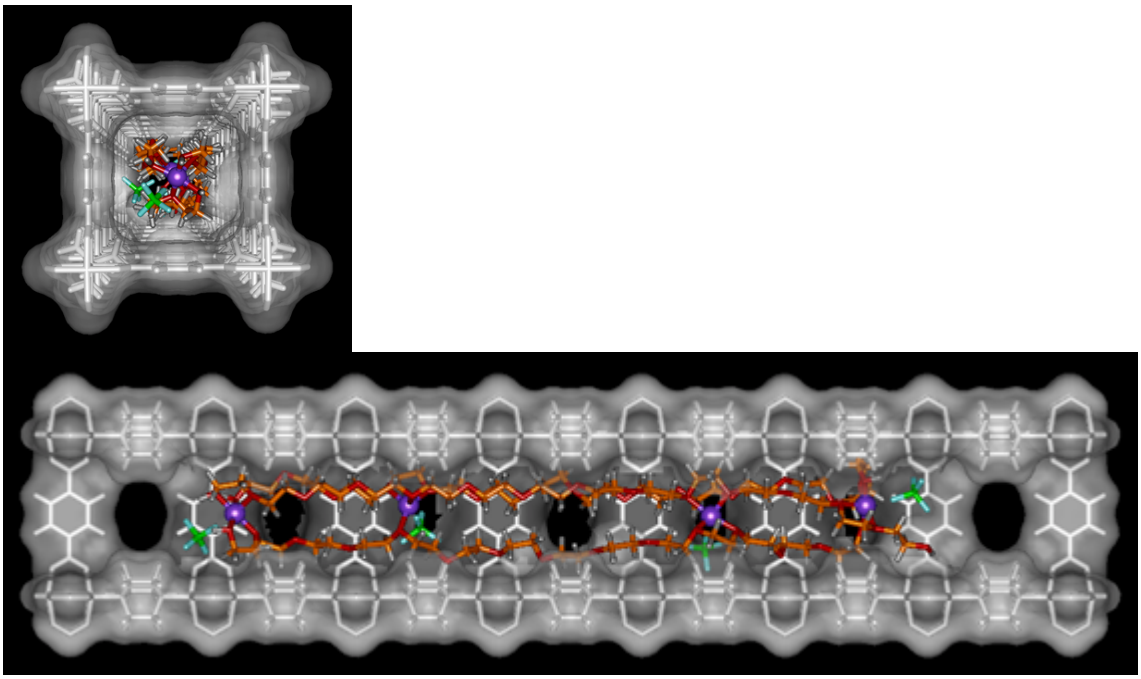

Fig. S4 Typical MD structure of PEG 14–mer (M_w = 634.7), Li^+, and BF_4^- encapsulated in the nanochannel of **1** at 25 °C (Li, purple; B, green; F, blue; C, orange; O, red; H, gray; host framework, white). The MD simulation was initially conducted by heating the model up to 1000 °C, followed by the cooling MD simulation down to 25 °C.

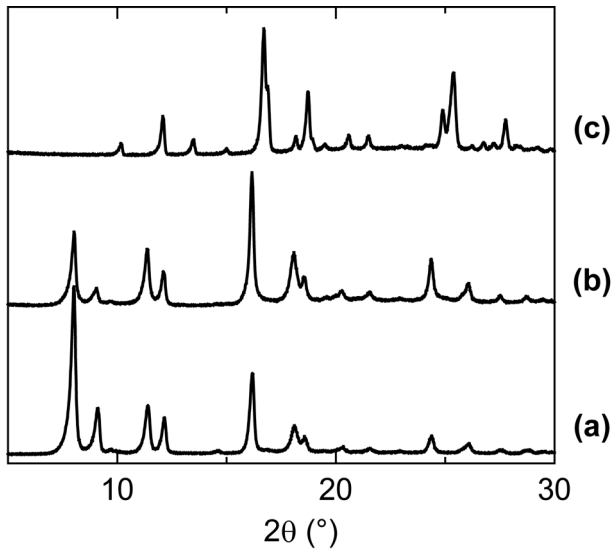

Fig. S5 XRPD patterns of (a) **1**⊃PEG(Li^+) and the sample obtained after exposing **1**⊃PEG(Li^+) to (b) air and (c) water vapor (100 % humidity) for 20 h. The crystalline host structure was intact in air, but the moisture treatment induced a transformation of the host structure to a totally different phase.

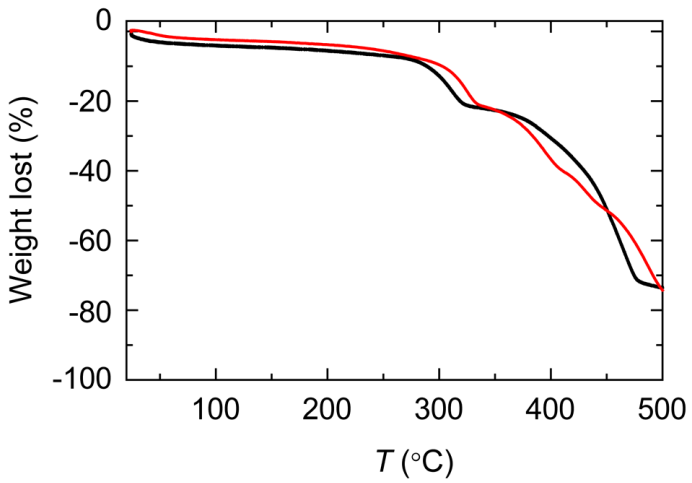

Fig. S6 Thermogravimetric analysis profiles of **1** (black) and **1**⊃PEG(Li^+) (red). The heating rate of the measurement was 10 K min^{-1}.