Supporting Information

Structure and Dynamic Behavior of Na-Diglyme Complex in the Graphite Anode of Sodium Ion Battery by ^{2}H NMR

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1) TEM images of pristine graphite and Na-diglyme-GIC

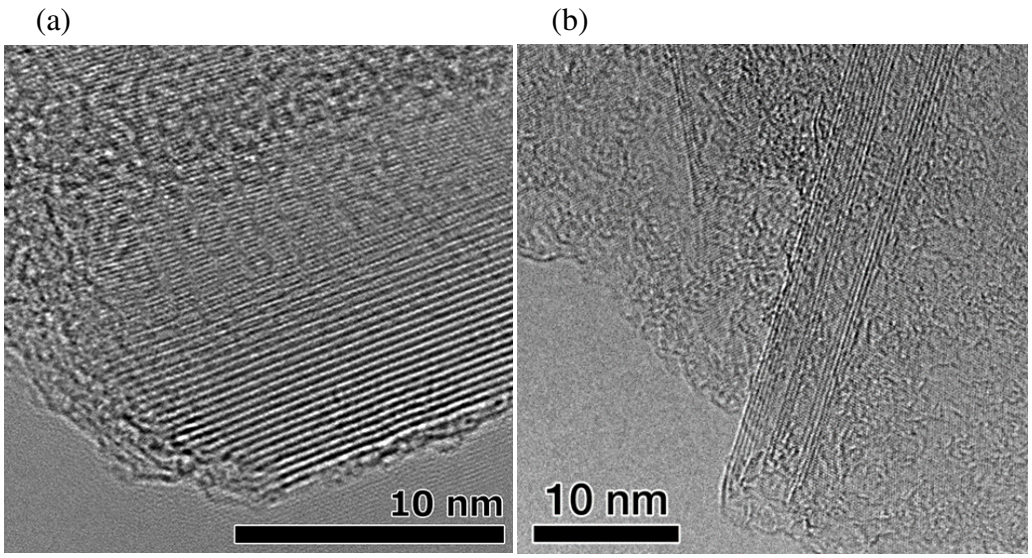

Figure S1. TEM images of pristine graphite (a) and Na-diglyme-GIC (b).

2) XRD patterns of Na-diglyme-GIC and Na-diglyme(d14)-GIC

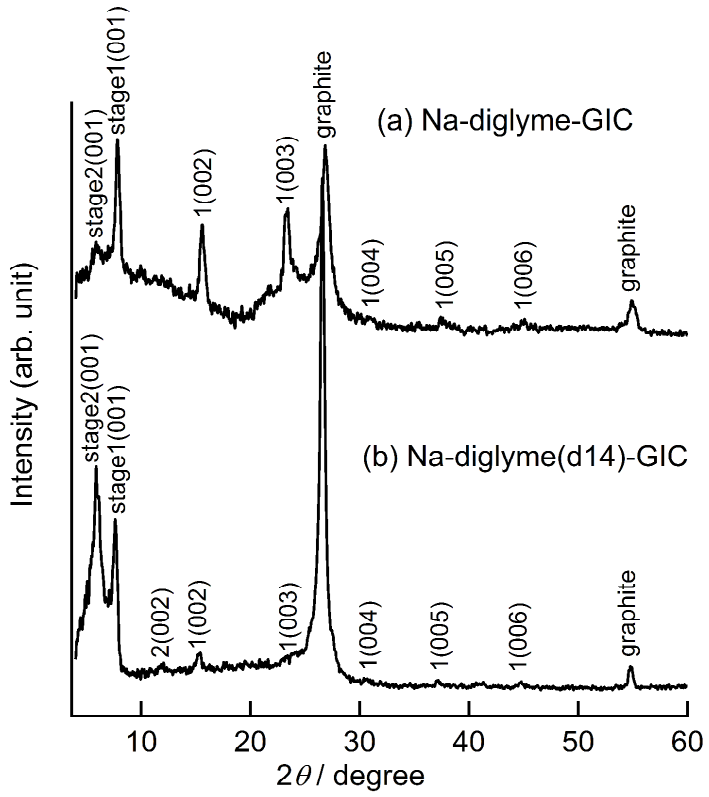

Figure S2. Powder XRD patterns of Na-diglyme-GIC (a) and Na-diglyme(d14)-GIC (b) synthesized using a solution-phase reaction. Both samples show peaks ascribed to stage 1 and stage 2 phases. The broad peaks around 5 and 27° in (a) are background reflections due to the sample holder window.

3) Composition of Na-diglyme-GIC

CHN elemental and ICP analyses were used to determine the composition of Na-diglyme-GIC. To obtain Na content by ICP, the GIC was rinsed by diglyme to remove Na on the surface of GIC sample and then combusted in air at 800 °C. The resulting ash (Na_2CO_3) was dissolved in ultrapure water. The mass not assigned to C, H, or Na was ascribed to oxygen.

Table S1. Results of elemental analysis and estimated composition of Na-diglyme-GIC

C	H	Na	O	composition
71.09±3.15	4.12±0.29	3.94±0.2	20.86	$C_{22\text{-}26}(\text{diglyme})_{1.8\text{-}2.2}Na_{1.0}$

4) ^{23}Na MAS NMR spectra of Na-diglyme-GIC

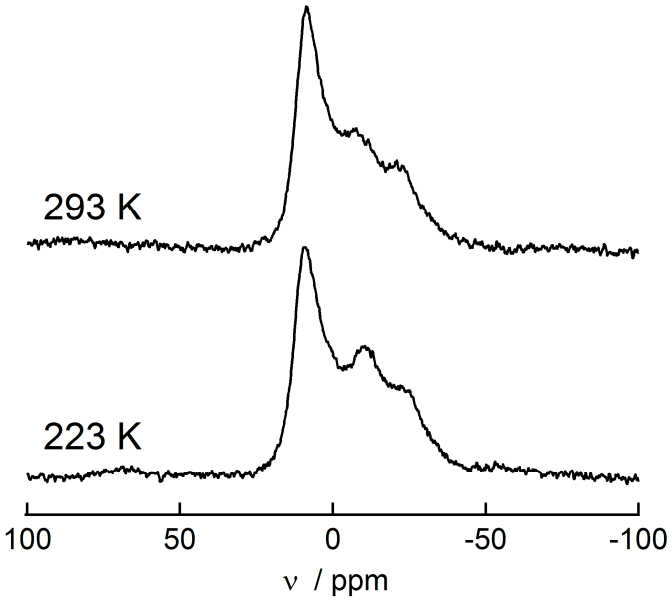

Figure S3. ^{23}Na MAS NMR spectrum of Na-diglyme-GIC taken at 293 and 223 K. Main peaks at 9 ppm and the edge structures at -25 ppm are ascribed to a predominant second-order quadrupolar component (quadrupolar coupling constant; qcc = 2 MHz) of sodium ion, whereas subordinate peaks at -9 ppm are assigned to sodium ion in diglyme liquid on the product surface or Na-diglyme located in defects in the GIC.

5) Schematic for the tilt of C–D bonds in CD_2 groups

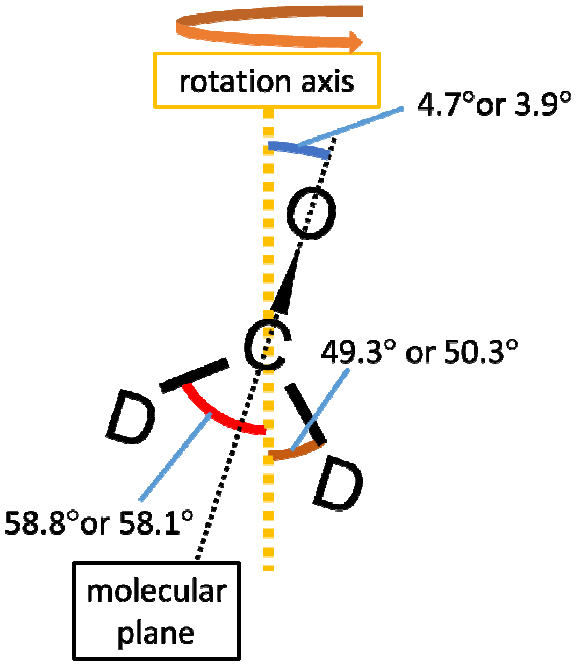

Figure S4. Schematic for the tilt of C–D bonds in CD_2 groups.