Electronic Supplementary Information

Tracking Rearrangement of Atomic Configurations During the Conversion from FAU zeolite to CHA zeolite

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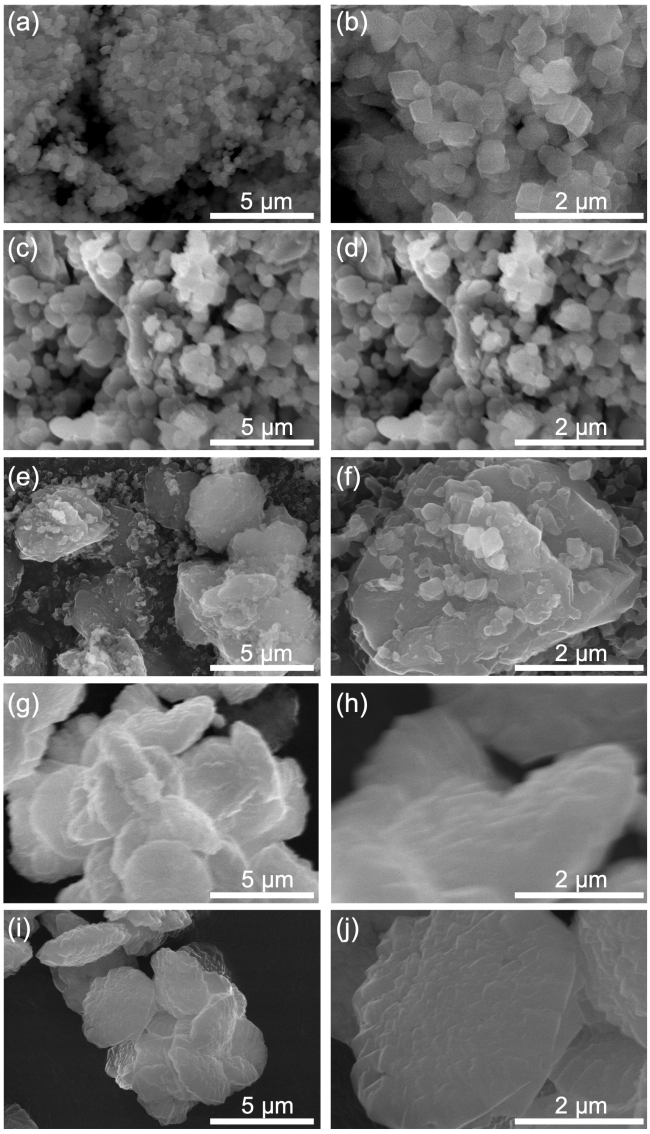

Fig. S1. SEM images of starting **FAU** (a, b), solid product after heating for 6 hours (c, d), solid product after heating for 8 hours (e, f), solid product after heating for 10 hours (g, h), and resulting **CHA** (i, j).

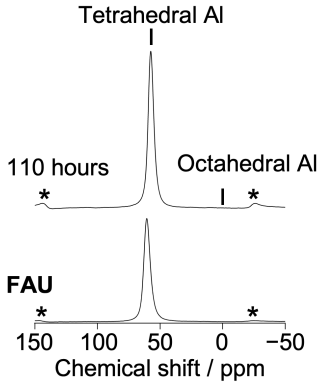

Fig. S2. ^{27}Al MAS NMR spectra of the starting **FAU** and product after heating for 110 h. *: Spinning side band.

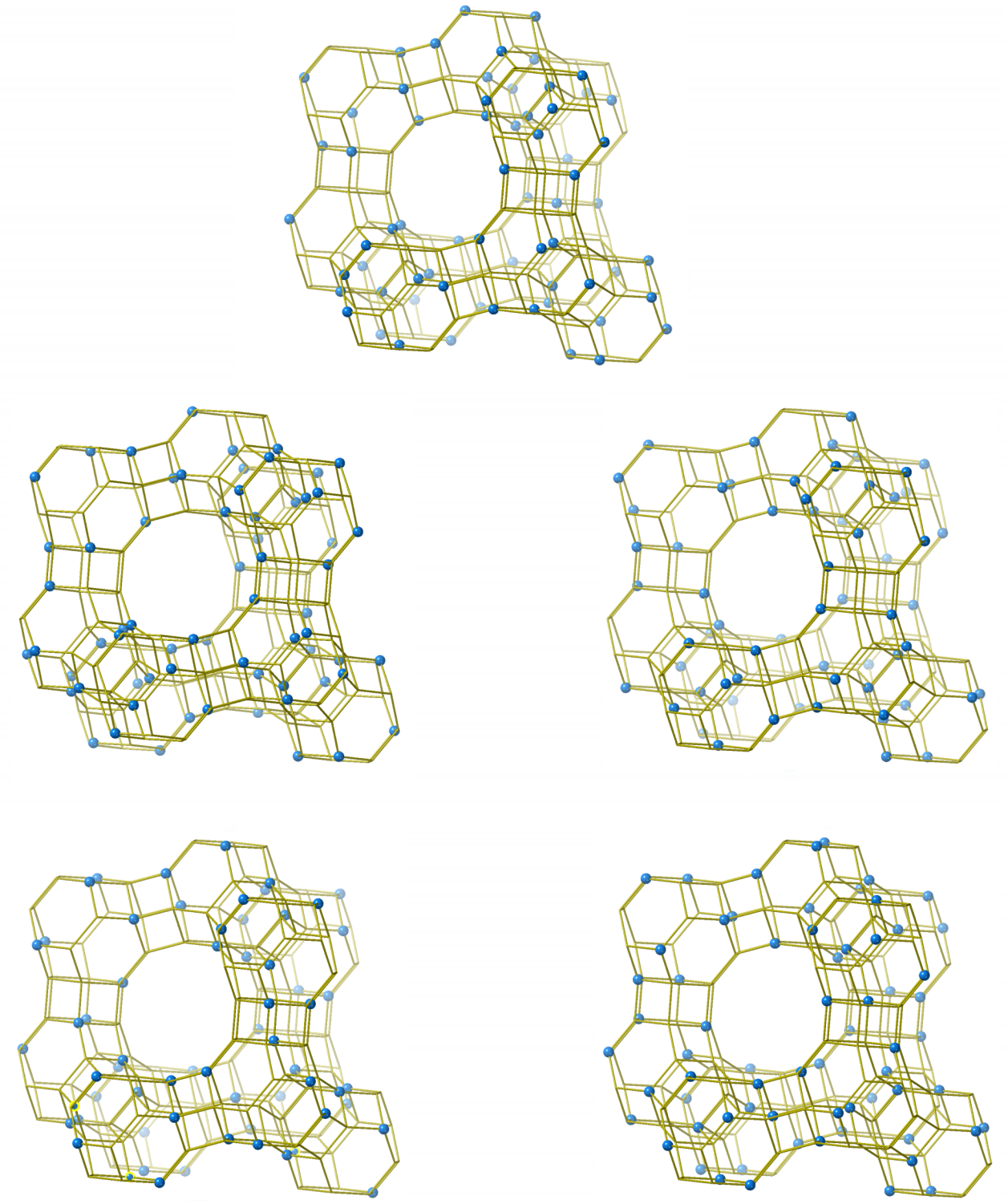

Fig. S3. Crystal structures of the five **FAU** models with Si/Al = 2.69 having $Q^4(n\text{Al})$ Si speciation closest to the starting **FAU**. Oxygen atoms are omitted for clarity. Aluminum atoms are shown as large blue spheres.

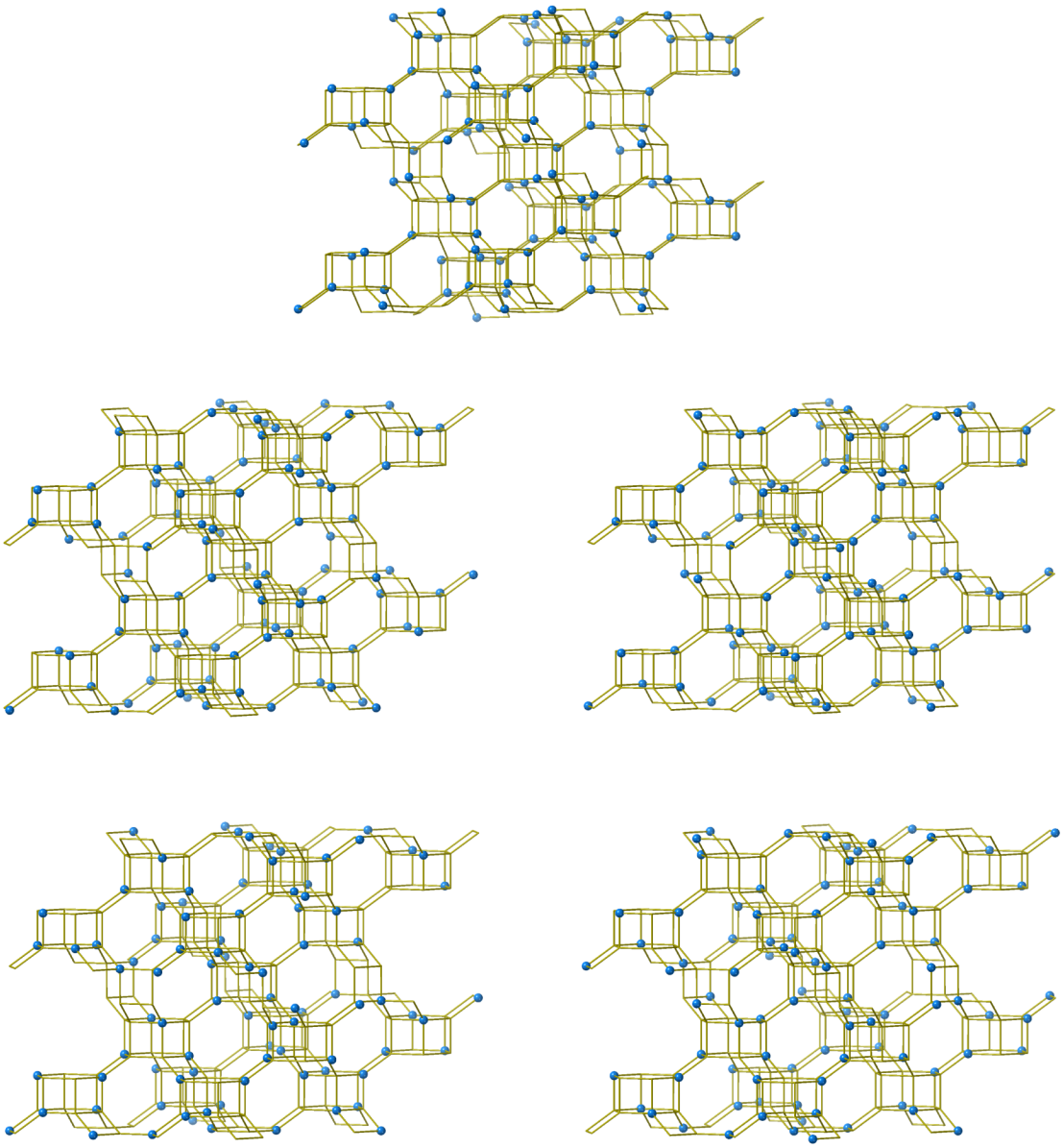

Fig. S4. Crystal structures of the five **CHA** models with Si/Al = 2.20 having Q^4(*n*Al) Si speciation closest to **CHA** synthesized from **FAU**. Oxygen atoms are omitted for clarity. Aluminum atoms are shown as large blue spheres.

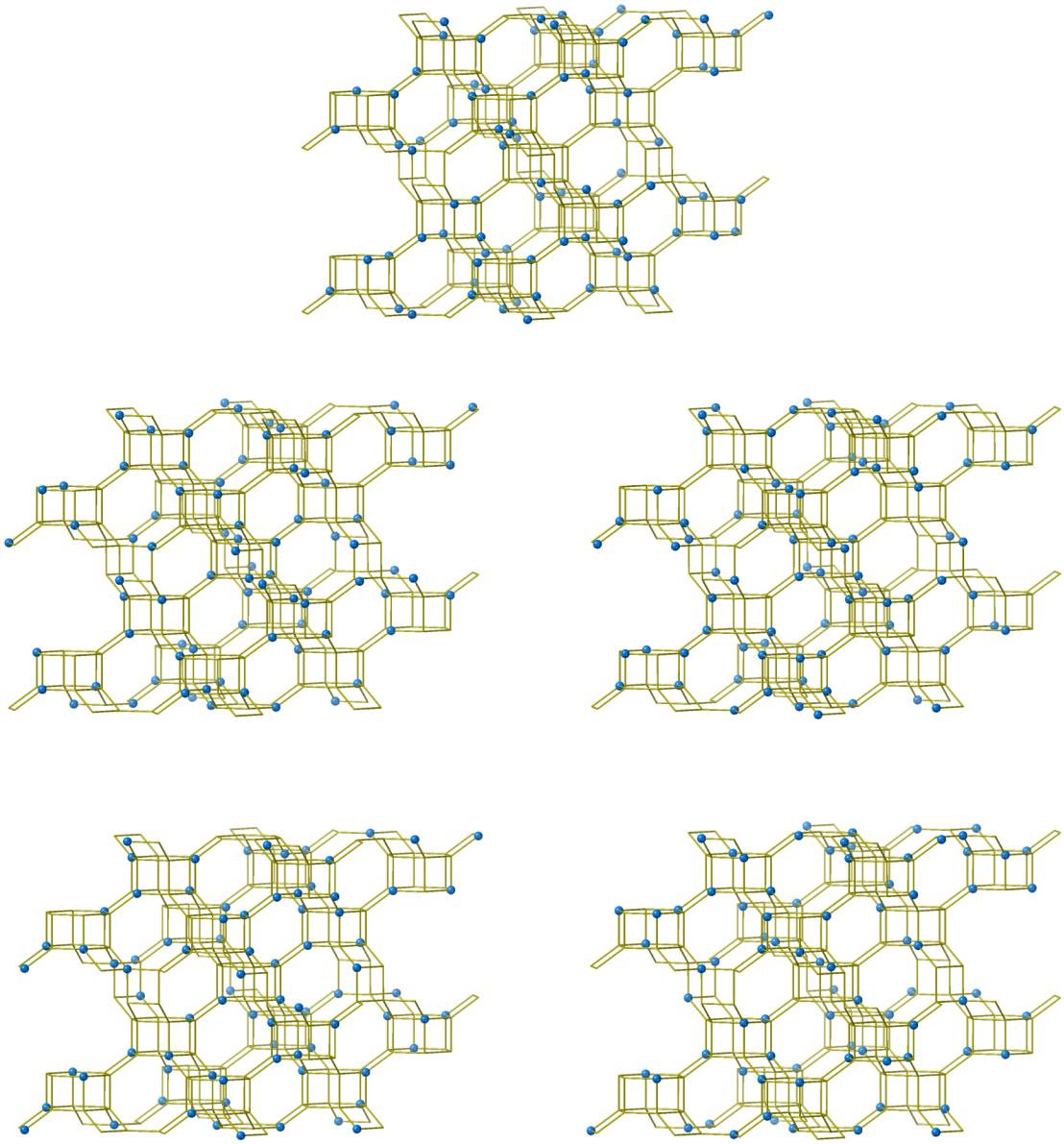

Fig. S5. Crystal structures of the five **CHA** models with Si/Al = 2.56 having $Q^4(n\text{Al})$ Si speciation closest to the previously reported **CHA**[1]. Oxygen atoms are omitted for clarity. Aluminum atoms are shown as large blue spheres.

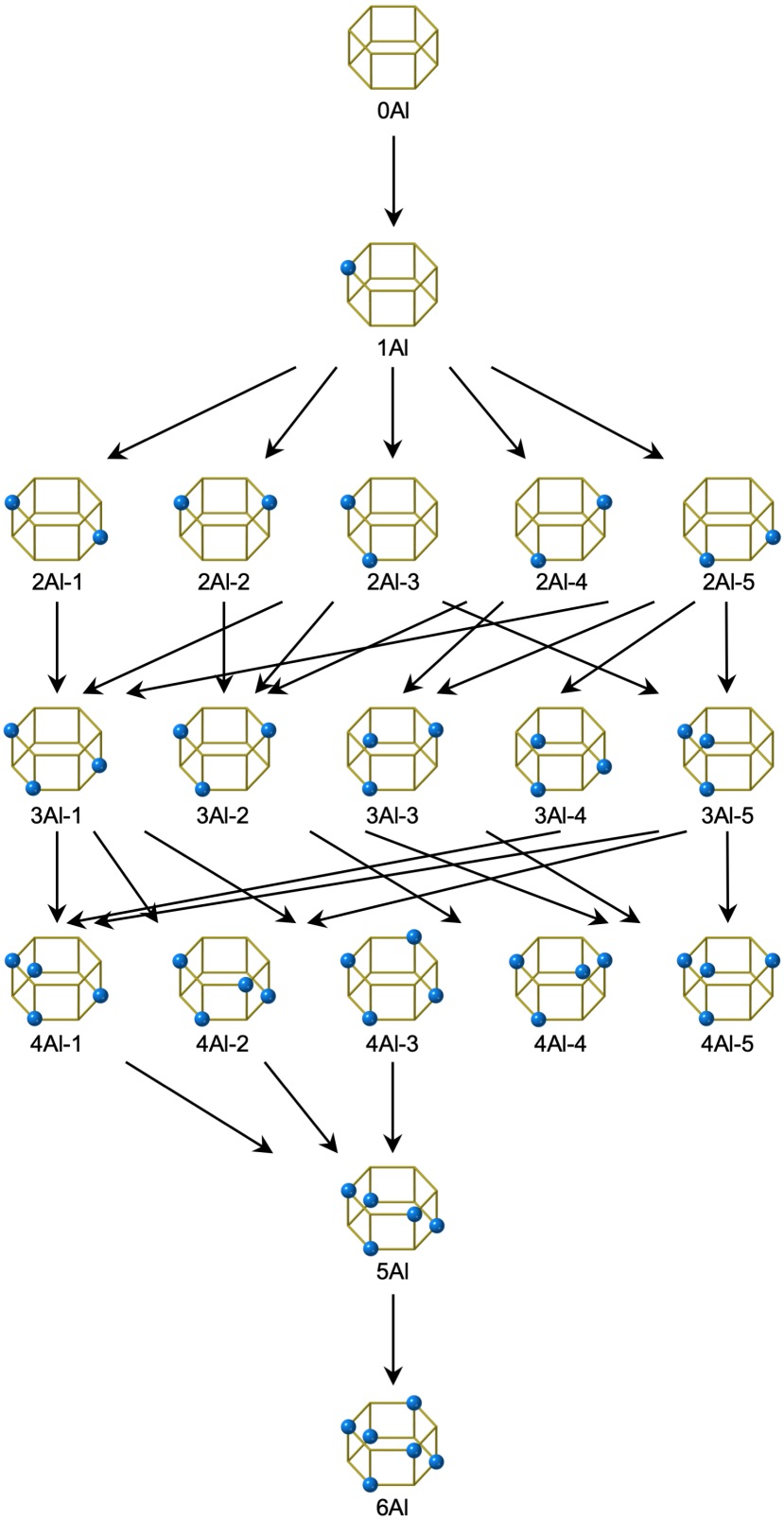

Fig. S6. Relationships between *d6r* species. An arrow connects a pair of *d6r* species that can be transformed by the isomorphic substitution between Si and Al.

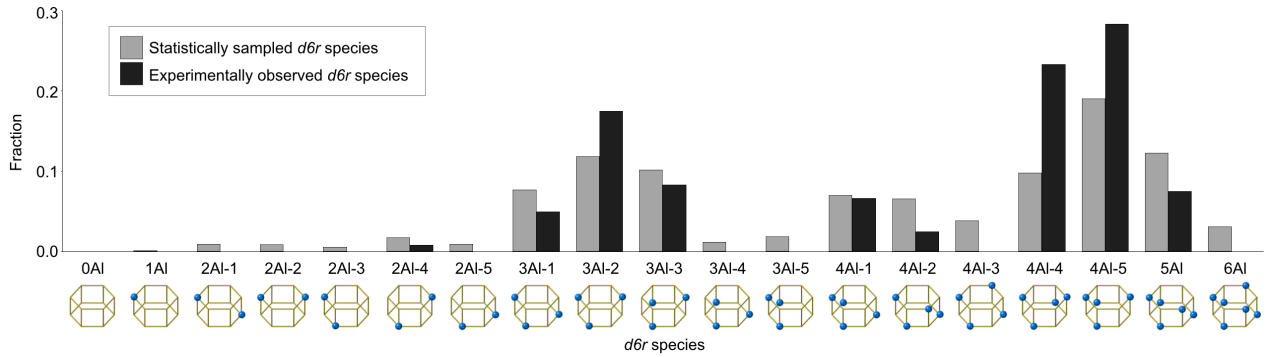

Fig. S7. Fractions and configurations of Al in the *d6r* units found in statistically sampled *d6r* species for **CHA** with Si/Al = 2.20 and **CHA** derived from **FAU**.

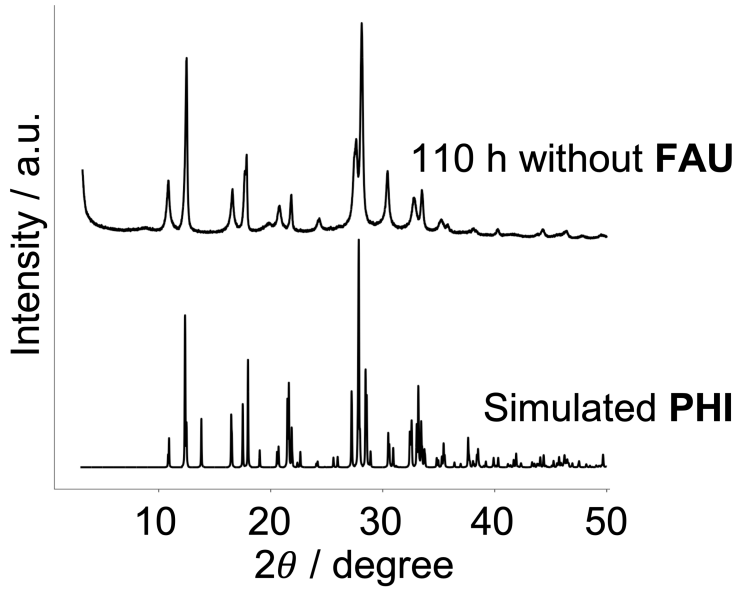

Fig. S8. Powder X-ray diffraction patterns of the sample synthesized with the same composition and heating time without using **FAU** as **CHA** synthesis from **FAU** in this work, and simulated patterns for **PHI**.[2]

References

(1) D. E. Akporiaye, I. M. Dahl, H. B. Mostad and R. Wendelbo, *J. Phys. Chem.*, 1996, **100**, 4148–4153.

(2) Database of Zeolite Structures, www.iza-structure.org/databases.