Supporting Information

Exploring Dehydration Mechanisms and Conductivity Optimization in $Li_3InCl_6 \cdot xH_2O$ via In-Situ Synchrotron Techniques

Jheng-Yi Huang,[a] Kevin Iputera,[a] Yen-Ting Lin,[a] Yuan-Ting Hung,[a] Yu-Shuo Liu,[a] Yun-Ping Chang,[a] Behrouz Bazri,[a,b] Bo-Hong Liu,[c] Da-Hua Wei[*,b] Bih-Yaw Jin [*,a] and Ru-Shi Liu*[*,a]*

[a] J. Y. Huang, K. Iputera, Y. T. Lin, Y. T. Hung, Y. S. Liu, Y. P. Chang, Prof. Dr. B. Y. Jin and Prof. Dr. R. S. Liu
Department of Chemistry and Advanced Research Center For Green Materials Science and Technology
National Taiwan University
Taipei 106, Taiwan
E-mails: byjin@ntu.edu.tw and rsliu@ntu.edu.tw
[b] B. Bazri and Prof. Dr. D. H. Wei
Institute of Manufacturing Technology and Department of Mechanical Engineering
National Taipei University of Technology
Taipei 106, Taiwan.
[c] Dr. B. H. Liu
National Synchrotron Radiation Research Center
Hsinchu 30076, Taiwan

Corresponding Authors

* Da-Hua Wei, Email: dhwei@ntut.edu.tw (D. H. Wei)

* Bih-Yaw Jin, E-mail: byjin@ntu.edu.tw (B. Y. Jin)

* Ru-Shi Liu, E-mail: rsliu@ntu.edu.tw (R. S. Liu)

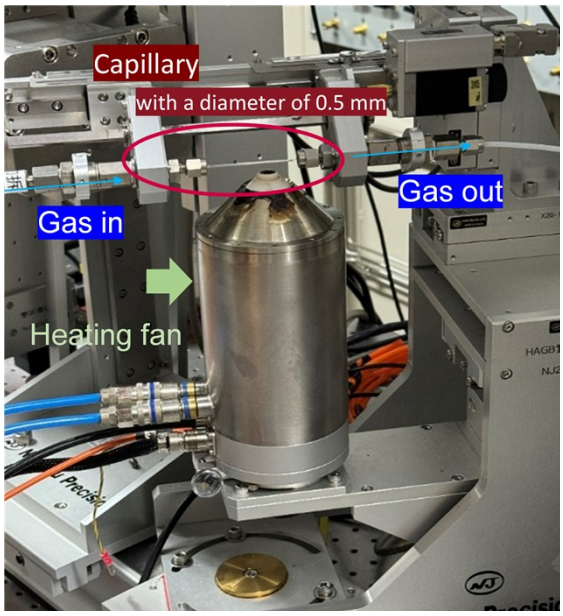

Fig. S1. The setup for *in-situ* XAS employs capillaries with a diameter of 0.5 mm in a nitrogen (N_2) environment.

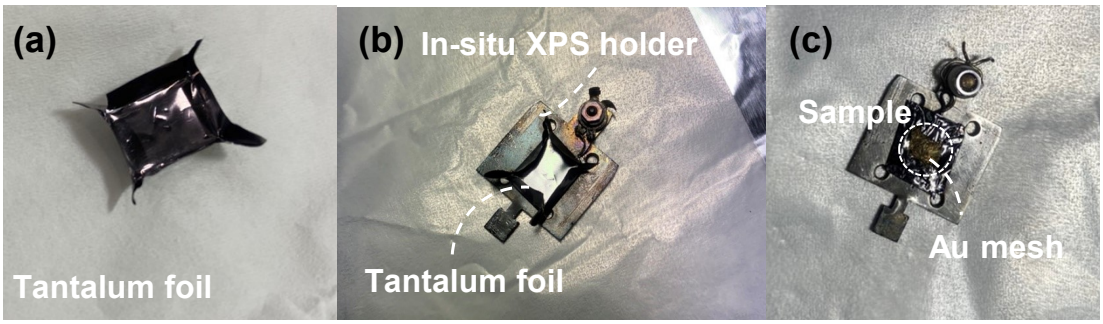

Fig. S2. (a)Tantalum (Ta) foil. (b) The *in-situ* XPS holder was welded with Ta foil. (c) The four sides of the holder can be folded to accommodate and secure the Au mesh.

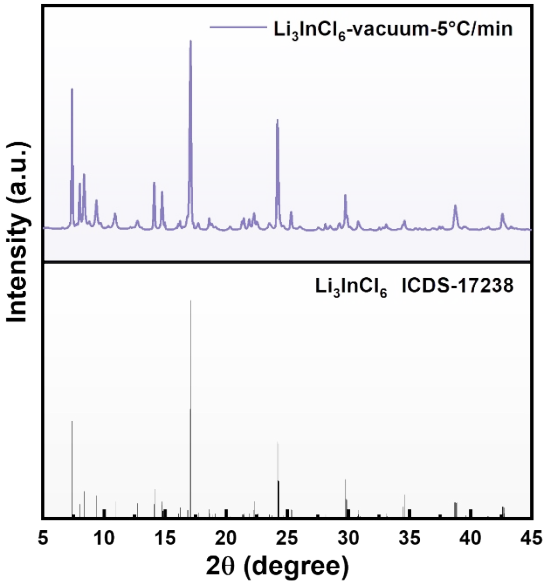

Fig. S3. XRD pattern of Li_3InCl_6 heat treatment at 200°C under vacuum for 5 h.

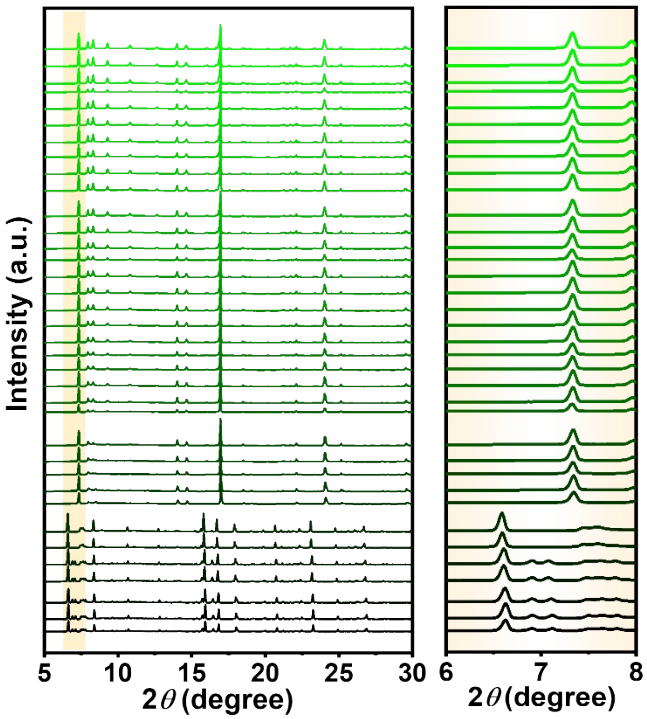

Fig. S4. *In-situ* XRD pattern of LIC-2H_2O heated at a rate of 20°C min^{-1} under Ar (1 atm).

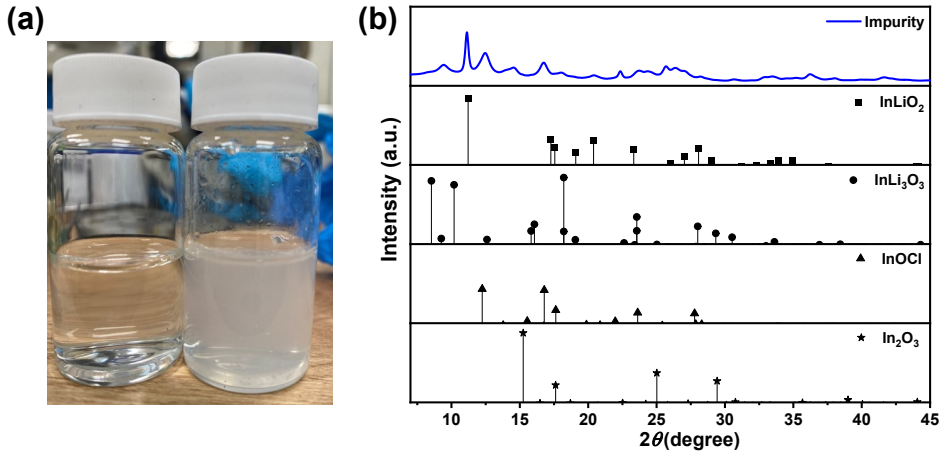

Fig. S5. (a) Photo of the precursor solution (left vial) and as-prepared LIC with optimized heat treatment dissolved into deionized water (right vial). (b) XRD pattern of white solid powder separated from the solution in the right-side vial of (a) by centrifugation.

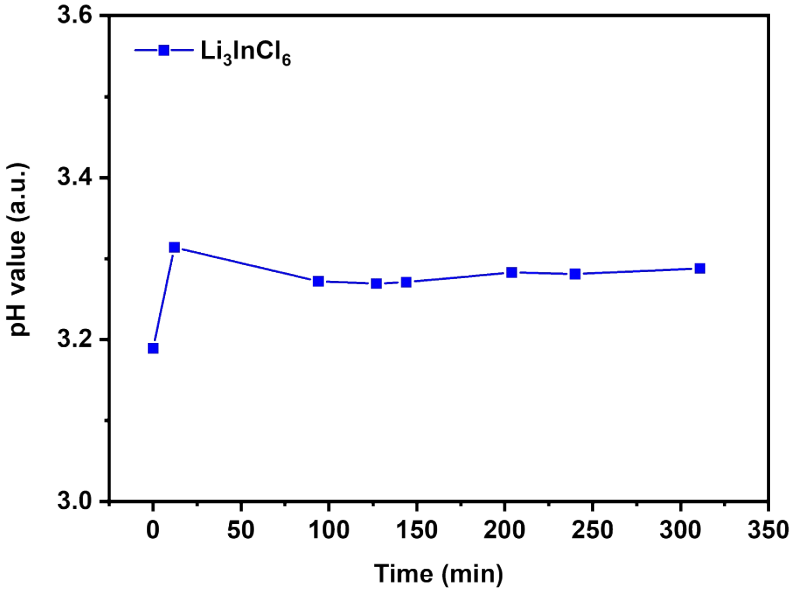

Fig. S6. The pH value of the precursor solution during different times.

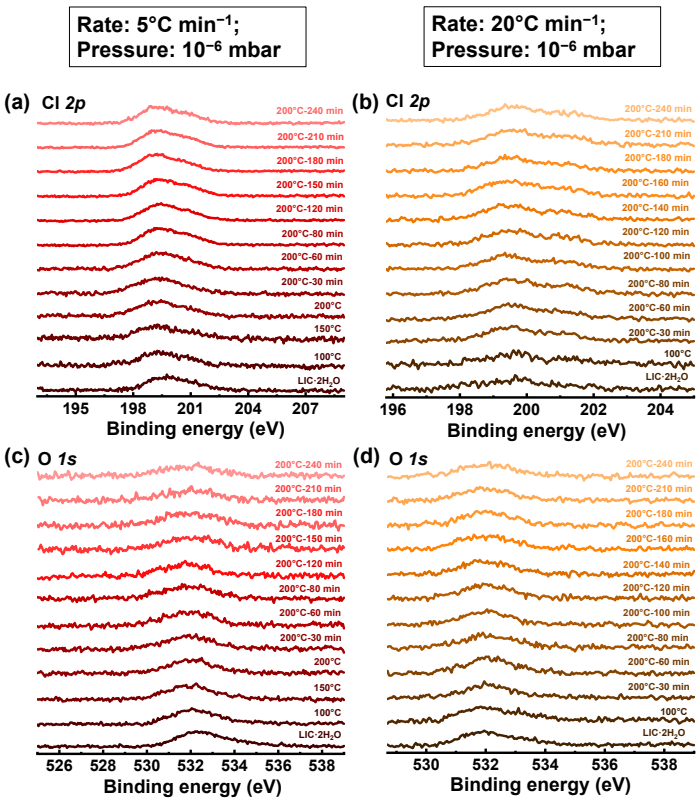

Fig. S7. Cl 2*p* (a,b) and O 1*s* (c,d) spectra of LIC-2H_2O throughout the heat treatment. The heat procedures in (a,b) and (c,d) are 5 °C min^{-1}-10^{-6} mbar and 20 °C min^{-1}-10^{-6} mbar, respectively.

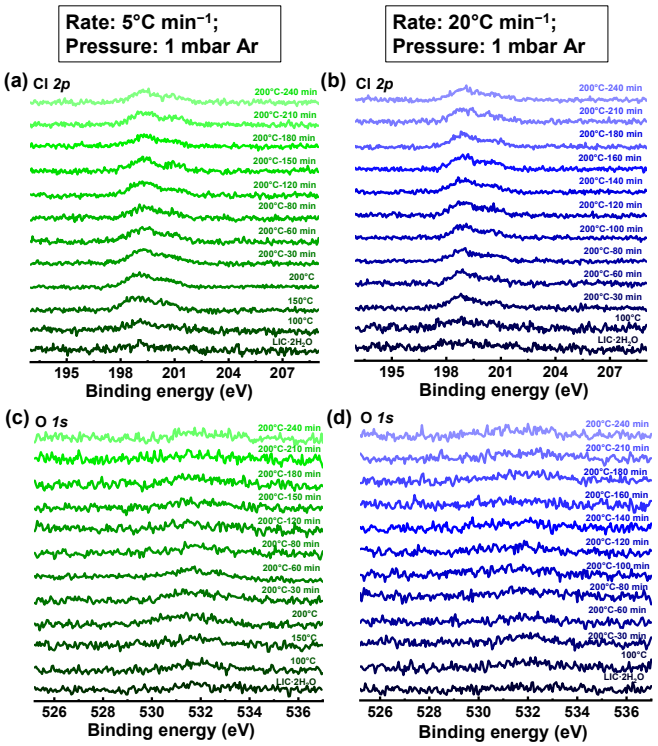

Fig. S8. Cl 2*p* (a,b) and O 1*s* (c,d) spectra of LIC-2H_2O throughout the heat treatment. The heat procedures in (a,b) and (c,d) are 5°C min^{-1}-1 mbar Ar and 20°C min^{-1}-1 mbar Ar, respectively.