A Functional Two-Dimensional Coordination Polymer Revives Li–S Batteries

The notorious sulfur-shuttling effect is suppressed with a functional 2D-coordination polymeric layer, which is a significant breakthrough in next-generation Li–S batteries.

Two-dimensional (2D) polymeric layers have become a fascinating research topic because of their unique physical properties by design and their potential applications in sensing, catalysis and energy conversion. Their ultrathin feature also enables a highly efficient separation of gases and molecules based on a commonly reported size-exclusion mechanism. In particular, ultrathin 2D polymeric layers are capable of separating gases and molecules based on that reported size-exclusion mechanism. What is equally important but missing at present is an exploration of the 2D layers with charge functionality, which enables applications using the charge-exclusion principle.

In the study done by Jing-Kai Huang (KAUST Solar Center) and his co-workers, a free-standing 2D-coordination polymer, namely, $Zn_2(benzimidazolate)_2(OH)_2$, was synthesized at the air–water interface, which improved the battery capacity and cycle performance.[1] The hydroxyl groups are stoichiometrically coordinated and implement electrostatic charges in the 2D-structures, providing powerful functionality as a charge barrier. The authors applied synchrotron-based grazing-incidence X-ray diffraction (GI-XRD) techniques at **TLS 23A1** to clarify the detailed structural information of layers of the zinc benzimidazolate coordination polymer (ZBCP) on water surfaces.

The GI-XRD reveals no evidence of a crystalline structure (**Fig. 1**), indicatng that the ZBCP layers might be amorphous in the in-plane direction. Because of this amorphous nature, there should be no well defined pore structures within the ZBCP; the porosity analysis consequently showed no pronounced porosity in the ZBCP. Furthermore, the amorphous structure increased the tolerance to mechanical stress relative to a crystalline film, which is advantageous for battery applications. This effect was inferred from the wrinkles but not cracks existing in the ZBCP thin film shown in SEM, OM and AFM images. The electrochemical performance of the Li–S battery shows that the $Zn_2(benzimidazolate)_2(OH)_2$ coordination polymer layers efficiently mitigate the polysulfide shuttling effects and greatly enhance the battery capacity and cycle performance.

In summary, a synthetic strategy was developed to grow a transferable Zn-coordination 2D-polymer of large area, in which hydroxyl groups and the amphoteric zinc hydroxides play an active role in the separation or selection according to the charge-exclusion principle. The charge-barrier feature has been integrated into the Li–S battery to mitigate the polysulfide shuttle effects by the electrostatic shield, greatly promoting the Li–S capacity and cycle performance. (Reported by Yan-Gu Lin)

*This report features the work of Jing-Kai Huang and his co-workers published in ACS Nano **12**, 836 (2018).*

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- SAXS, WAXS
- Soft Matter, Protein Crystallography, Materials Science, Atomic and Molecular Science

Reference

1. J.-K. Huang, M. Li, Y. Wan, S. Dey, M. Ostwal, D. Zhang, C.-W. Yang, C.-J. Su, U.-S. Jeng, J. Ming, A. Amassian, Z. Lai, Y. Han, S. Li, L.-J. Li, ACS Nano **12**, 836 (2018).

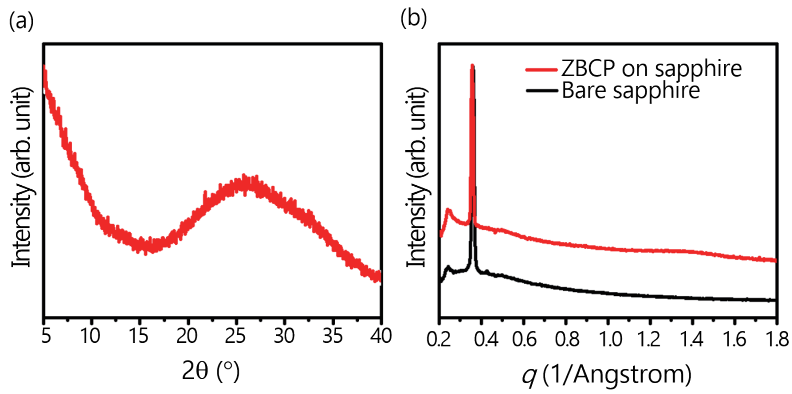

Fig. 1: (a) XRD profile with a broad amorphous halo and (b) GI-XRD profiles exhibiting only the crystalline peak from the sapphire substrate; these features indicate the non-crystalline nature of the film. [Reproduced from Ref. 1]