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# Structural Design of 2D Materials for Energy Storage

Several examples are given here for the work carried out in CA2DM concerning the design and synthesis of 2D Materials for Energy Storage, ranging from $MoS_2$ to 2D polymer.

There have been a lot of interests on the phase engineering of transition metal dichalcogenides for applications in catalysis and energy storage. For example converting the 2H to 1T phase in $MoS_2$ has been credited with improvement in conductivity and catalytic activities. Here we demonstrate that the 2H phase can also be used in catalysis if proper materials design is carried out [1]. Instead of exfoliating 2D sheets from a bulk, layered 2D materials, bulk 2D materials can be intercalated with alkali metal ions to become a quasi-2D material. We exploited the highly reductive, lithiated host materials ($Li_xMoS_2$) to reduce ion precursors to zero valent metal (Fig. 1). This provides a strong driving force to overcome van der Waals interactions and transforms the quasi-2D materials into a unique, $MoS_2$ | noble metals | $MoS_2$ sandwich. We further demonstrated industrial scalability by fabricating a 25 $cm^2$ catalyst-loaded water splitting membrane. The synergetic host–guest interaction also allows ultra-stable, long-term operation in hydrogen production with a reduced metal loading compared with commercial catalyst. This concept of confinement by 2D materials can potentially be applied to various catalytic reactions and many other energy-related applications.

Sulfur-lithium battery is highly promising for energy storage but the dissolution of its lithiated product (lithium polysulfides) into the electrolyte limits the practical application of lithium sulfur batteries. Here we demonstrate that sulfur particles can be hermetically encapsulated by leveraging on the unique properties of two-dimensional materials such as molybdenum disulfide ($MoS_2$) (Fig. 2). The high flexibility and strong van der Waals force in $MoS_2$ nanoflakes allows effective encapsulation of the sulfur particles and prevent its sublimation during *in situ* TEM studies [2]. We observe that the lithium diffusivities in the encapsulated sulfur particles are in the order of $10^{-17}$ $m^2$ $s^{-1}$. Composite electrodes made from the $MoS_2$-encapsulated sulfur spheres show outstanding electrochemical performance, with an initial capacity of 1660 mAh $g^{-1}$ and long cycle life of more than 1000 cycles.

The synthesis of graphene-like, conjugated aromatic 2D polymer is one of the greatest challenges in synthetic chemistry. We have successfully synthesized a crystalline 2D conjugated aromatic polymer (2D-CAP) by topochemical polymerization of a molecular crystal based on C-C coupling between adjacent monomers [3]. 2D-CAP crystalline polymer has a layered stacking structure and can be readily exfoliated into ultrathin sheets. 2D-CAP also has highly ordered porosity (pore size 6 Å) created by the stacking of slightly slipped 2D-CAP sheets. Due to its intrasheet conjugation and ordered open 1D channels, 2D-CAP exhibits unpredecented cycle stability and rate capability when applied as an anode in an ambient temperature sodium battery cell. When applied as an asymmetric supercapacitor, it delivers a specific capacitance of 233 F $g^{-1}$ at a current density of 1.0 A $g^{-1}$ with outstanding cycle performance. The topochemical C-C coupling polymerization approach presented here opens a new avenue for constructing novel 2D polymers with highly regular porosity and chemical stability, which is currently a major challenge in synthetic chemistry.

## References


[1] Zhongxin Chen, Kai Leng, and Kian Ping Loh et. al., NATURE COMMUNICATIONS 8 (2017) 14548.
[2] Wei Tang, Zhongxin; Kian Pingf Loh, Guangyuan Zheng et. al., JACS, 139 (2017) 10133–10141.
[3] Wei Liu and Kian Ping Loh et. al., NATURE CHEMISTRY 9 (2017) 563–570.
[4] Peng, Chengxin and Kian Ping Loh et. al. NATURE ENERGY 2 (2017) 17074 .


## Figures

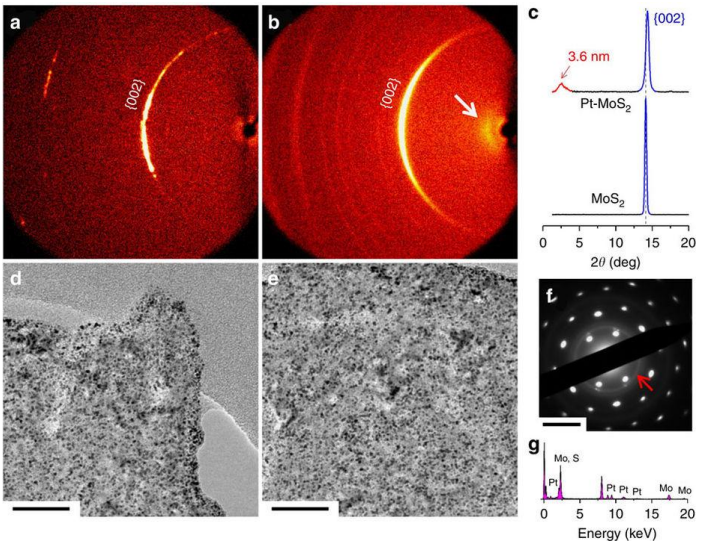


**Figure 1: Pt-coated quasi-2D MoS2 shows highly stable performance in hydrogen evolution reactions.**

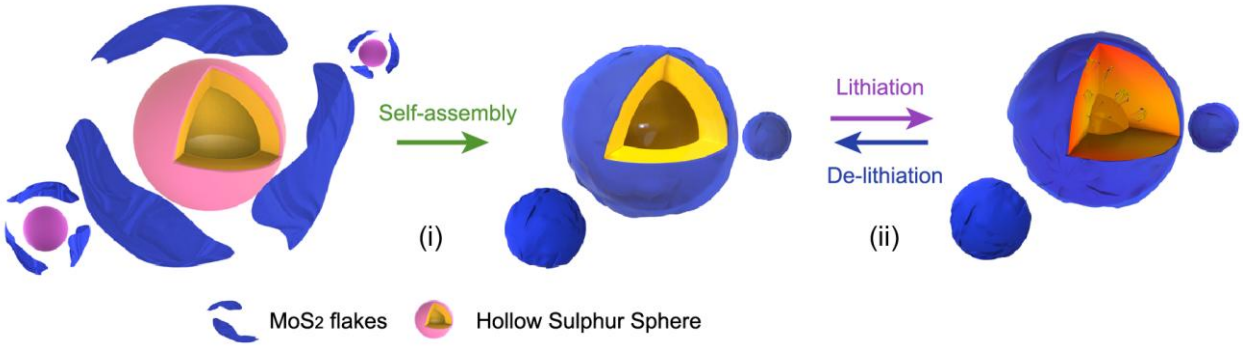


**Figure 2: Hermetic encapsulation of sulfur particles by MoS2 flakes protects it from chemical corrosion during battery applications.**