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Precise synthesis of 2D crystals for energy applications

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Layered transition metal dichalcogenides (TMDs) display a variety of structural polymorphs defined by the symmetry of transition metal coordination polyhedra. Tailoring the lattice symmetry within individual TMD layers enables to achieve very different electronic properties ranging from semiconducting (2H phase) to metallic and semimetallic (1T/1T' phases) with the same material composition. Exhibiting metallic behaviour, the metastable 1T' phases are particularly appealing for electrocatalytic hydrogen production from acid water as they approach Pt performance. The direct synthesis of the metastable phases of high purity and in measurable quantities remains challenging. Here, we present our work on the bottom-up synthesis of the metastable 1T' phase of WSe_2 based on the reaction between molecular precursors in liquid phase [1]. We design a kinetically-controlled bottom-up synthesis from molecular precursors to enable the formation of the metastable phase. We further demonstrate that the 1T' phase is stable up to 400 ^{o}C and it is convertible into the semiconducting 2H phase at higher temperatures, making it suitable for a wide range of applications. The 1T' WSe_2 nanosheets exhibit a metallic nature evidenced by an enhanced electrocatalytic activity for hydrogen evolution reaction as compared to the 2H WSe_2 and different sulphides. Further, we demonstrate how this synthesis approach can be applied to design of new catalytic systems.

References

[1] M. S. Sokolikova, P. C. Sherrell, P. Palczynski, V. L. Bemmer and C. Mattevi, *Nat. Commun.*, 2019, **10**, 712].