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One-step Efficient Preparation of Unconventional Phase of Transition Metal Dichalcogenides

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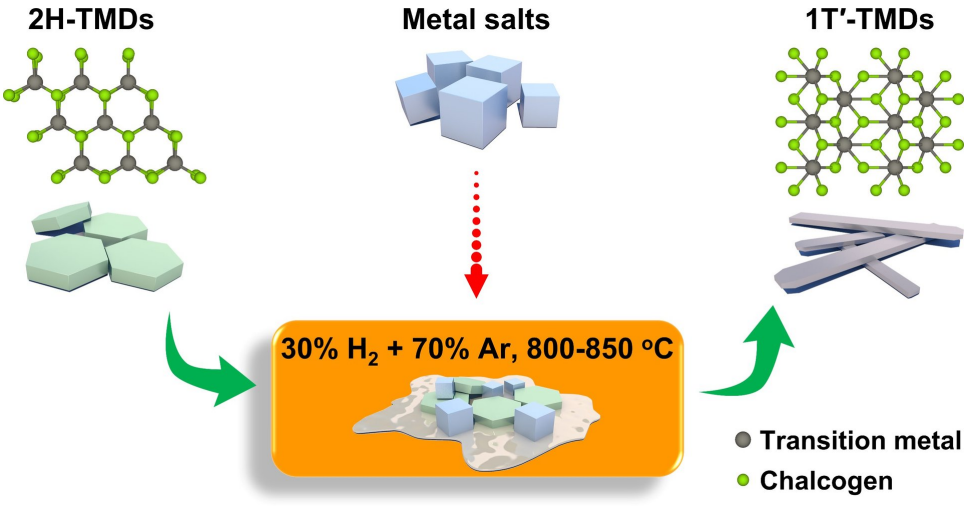

Figure 1. Schematic illustration of the general strategy for the phase transformation of TMDs (WS_2, WSe_2, MoS_2 and $MoSe_2$) from 2H to 1T′ phases assisted by various types of salts, such as $K_2C_2O_4{\cdot}H_2O$, K_2CO_3, Na_2CO_3, Rb_2CO_3, Cs_2CO_3, $KHCO_3$, $NaHCO_3$, and $Na_2C_2O_4$.

IP Status
Patent filed

Technology Readiness Level (TRL) ? 5

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Opportunity

The phases of transition-metal dichalcogenides (TMDs) play an important role in determining the intrinsic properties of TMDs, and thus their various applications. For example, TMDs with unconventional metastable phases (e.g., 1T and 1T′) have novel physical and chemical properties and hold great potential applications in electronic devices, energy storage and conversion, catalysts, and condensed matter physics. Meanwhile, most of the known methods to prepare metastable-phase TMDs require either harsh conditions or destructive treatment, resulting in damages and defects on TMDs during the preparation process, which are not suitable for the large-scale production of high-quality metastable-phase TMDs. The large-scale preparation of metastable-phase TMDs with high quality and purity remains challenging. The present invention offers a simple, universal, and controlled method for the preparation of large-scale and high-purity unconventional-phase TMDs from the easily accessible and low-cost 2H-phase TMDs and alkali metal, which will benefit the research on the fundamental study of these unconventional-phase TMDs and the phase-dependent applications.

Technology

The present technology relates to a simple, facile, and general salt-assisted synthetic method for the preparation of a series of unconventional 1T′-phase transition metal dichalcogenides (TMDs). In this synthetic method, easily accessible ingredients of commercialized 2H-phase TMDs (e.g. 2H-phase WS_2, 2H-phase WSe_2) and alkali metal salt were mixed uniformly and then heated at high temperature under the mixed gas flow of hydrogen (H_2) and Argon (Ar) to prepare the desired 1T′-phase TMDs. The alkali metal salt is critical for the phase transformation. This method involves a one-step gas-solid reaction for phase transformation from 2H to 1T′, which is simple and efficient. At least 6 types of unconventional 1T′-phase TMDs, including WS_2, WSe_2, MoS_2, $MoSe_2$, $WS_{2x}S_{2(1-x)}$ and $MoS_{2x}S_{2(1-x)}$, have been prepared, which demonstrates high universality, high yield and simplified direct phase transformation process. Importantly, the unconventional 1T′-phase TMDs are applicable in electrocatalysis (e.g., CO_2 reduction reaction and hydrogen evolution reaction), energy storage (supercapacitors) and condensed matter physics (e.g., superconductivity).

Advantages

- Efficient and simplified one-step gas-solid reaction
- Reduced the production cost
- High purity and controllability

Applications

- Catalysis (e.g., CO_2 reduction reaction and hydrogen evolution reaction)
- Energy storage and conversion (e.g., battery and supercapacitors)
- Electronic devices
- Condensed matter physics