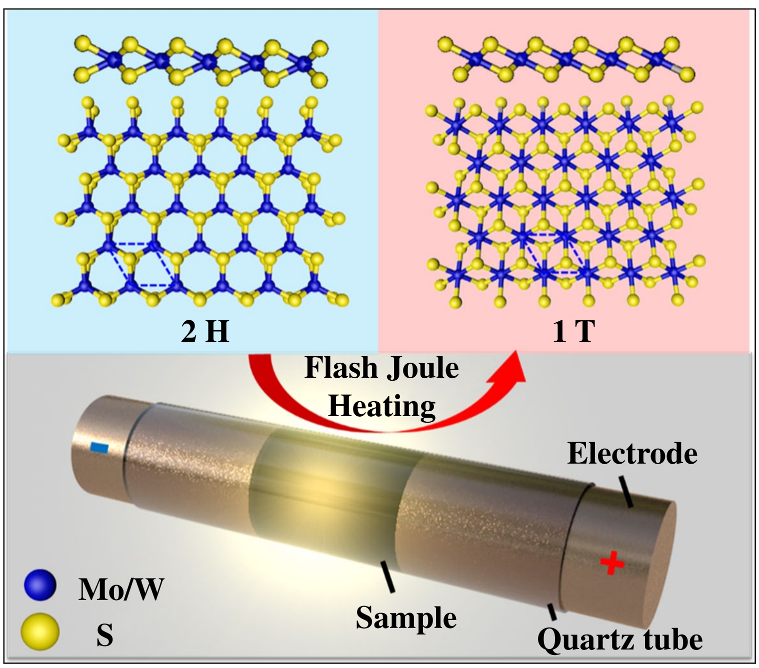
Metastable 2D materials synthesized with flash Joule heating

The synthesis of two-dimensional (2D) metastable materials remains challenging. As reported in a recent issue of *ACS Nano* (https://doi.org/10.1021/acsnano.0c08460), James M. Tour, Boris I. Yakobson, Weiyin Chen, and colleagues at Rice University realized that flash Joule heating (FJH), which is an electrothermal method, can be used to achieve bulk conversion of transition-metal dichalcogenides, such as MoS_2 and WS_2, from 2 H phases where the transition metal has trigonal prismatic coordination (space group $P6_3/mmc$) to 1 T where the transition metal octahedrally coordinated (space group $P\bar{3}m$) phases in milliseconds. FJH provides short electrical pulses of high energy density followed by rapid cooling inducing the bulk conversion. Chen—first author of the article—told *MRS Bulletin,* "During the flash process, the energy is released within milliseconds and the bulk quantities of powder samples can be synthesized. The yield of metastable materials can be controlled by the reaction durations and the types of conductive additives, which offers a straight strategy to synthesize metastable materials controllably."



Schematic diagram of the phase conversion via flash Joule heating. The inset shows the atomic structure of the 2 H and 1 T phases from the side and top view. Credit: *ACS Nano.*

According to Chen, the research team initially found the metastable phases by accident. "When I took the Raman spectra of the MoS_2 after the flash reaction for the first time, I chose a range from 300 to 500 cm^{-1}, since I knew there should be two peaks at ~380 cm^{-1} (E_{2g}) and ~405 cm^{-1} (A_g). But to my surprise there was one more peak at ~335 cm^{-1}," he says. Realizing that the peak may represent the metastable phase of MoS_2, they conducted additional experiments and subsequently did simulations to confirm their findings. "The flash Joule heating method, which essentially [is] an electrothermal method, can provide short electrical pulses of high energy density followed by rapid cooling," Chen says. "[It] has the potential to induce the formation of materials with metastable phases, since there is not enough time for the atoms and molecules to move to thermodynamically most stable positions."

According to the research group, FJH is a fast, simple method that can achieve bulk conversion. The first-principles density functional theory calculations reveal that the high current and large energy input result in the formation of structural defects such as S vacancies and the negative charge buildup leading to the thermodynamic preference toward the metastable 1 T phase in FJH. An advantage of this technique is that it offers the possibility of a promising method with high temperature and rapid cooling rate to synthesize bulk quantities of metastable materials, which is valuable for fundamental research and diverse applications.

J. Arnaldo Méndez-Román