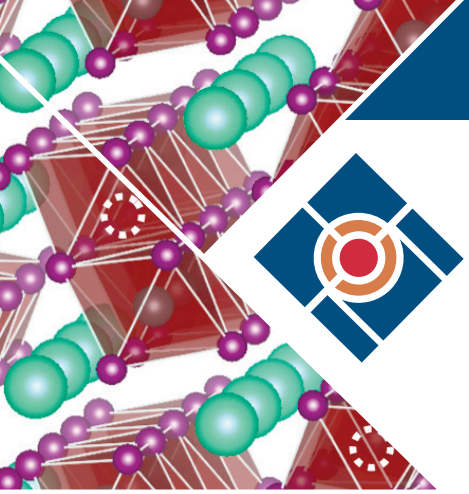

Understanding phase transition dynamics paves the way to halide perovskites nanoelectronics

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Structural phase transitions in semiconductors have been utilized for driving technological advancements in switchable electronics and phase-change memory devices. There have been numerous reports on high susceptibility of halide perovskites to phase transitions because of their soft lattice; however, the factors affecting the underlying process are still poorly understood. Insights into the phase transition dynamics of halide perovskites are desirable for precise control of optoelectronic properties and for unlocking their use in novel solid-state applications.

The article by Lai et al.[1] reports on a systematic evaluation of the phase transition dynamics between low-temperature (low-T) and high-temperature (high-T) phases of $CsSnI_3$ and $FAPbI_3$ nanowires. Their quantitative estimation reveals a lower kinetic energy barrier for non-perovskite (low-T) to perovskite (high-T) phase transition in $FAPbI_3$ owing to the relatively smaller activation energy in $FAPbI_3$ (~0.84 eV) compared to $CsSnI_3$ (~1.93 eV).[1]

The solid-solid phase transitions triggered by thermal energy, electric field, optical excitation, and strain have been extensively studied in metal oxides, transition metal dichalcogenides, and GeSbTe alloys.[2] The contrast in electrical and optical properties offered by phase engineering of these materials has led to the fabrication of innovative functional devices. Electrochromic smart windows have been demonstrated using the metal-insulator transition in VO_2 films.[3] Cho et al. has fabricated a high mobility transistor by realizing a laser irradiation-induced homojunction between metal-semiconductor phases of $MoTe_2$.[4] The amorphous to crystalline phase change due to Joule heating of $Ge_2Sb_2Te_5$ nanowires has been used for non-volatile memory devices.[5] One of the latest additions to these phase-change materials are halide perovskites, which have gained tremendous attention in the last decade because of their exceptional optoelectronic properties. However, unlike their counterparts, the relative ease of phase transition in halide perovskites is typically considered undesirable due to its detrimental impact on long-term stability.[6] Insights about the thermodynamics of phase transitions between different halide perovskite polymorphs will not only tackle the perovskite stability issue but will also open up opportunities for novel solid-state applications.

To investigate the phase transition dynamics in halide perovskites, Lai et al.[1] employed non-invasive *in situ* optical microspectroscopy. They chose two model systems—$CsSnI_3$ and $FAPbI_3$—to study the impact of crystal structure and defect types on phase transition and phase propagation. Using thermal activation followed by quenching, a partial phase transition and heterojunction formation was obtained in $FAPbI_3$. Compared to the high-T perovskite phase, a significant blue-shift (~38 meV) in photoluminescence spectrum is observed at the two-phase heterojunction. Interestingly, the origin of increased band gap at heterojunction is attributed to lattice distortion because of octahedral titling at the boundary of face-sharing non-perovskite and corner-sharing perovskite phases. The presence of Sn vacancies in $CsSnI_3$ leads to approximately three orders of magnitude higher phase propagation rate compared to ion-diffusion-mediated phase growth in previously reported $CsPbBr_2I$.[7] Temperature-dependent phase propagation rate is used to estimate the activation energy barrier for phase transition. **Figure 1** compares the calculated activation energy barriers for phase transition in $FAPbI_3$ (~0.84 eV), $CsSnI_3$ (~1.93 eV), and $CsPbBr_2I$ (~2.18 eV).[7] This indicates that the face-sharing to corner-sharing phase transition in $FAPbI_3$ offers a much smaller energy barrier compared to edge-sharing to corner-sharing phase transitions for $CsSnI_3$ and $CsPbBr_2I$.

Through their research, Lai et al.[1] highlight the governing role of crystal structure and inherent vacancies in phase transition of halide perovskites. Precise controlling of phase transition dynamics can be used to locally change the crystal structure and improve intrinsic material properties. For instance, epitaxial stabilization and strain neutralization have already been employed for demonstrating the enhanced performance of $FAPbI_3$-based photodetectors.[8] Phase engineering can also be used for fabrication of high-quality perovskite-based heterojunctions with potential applications in new functional devices.[9,10]

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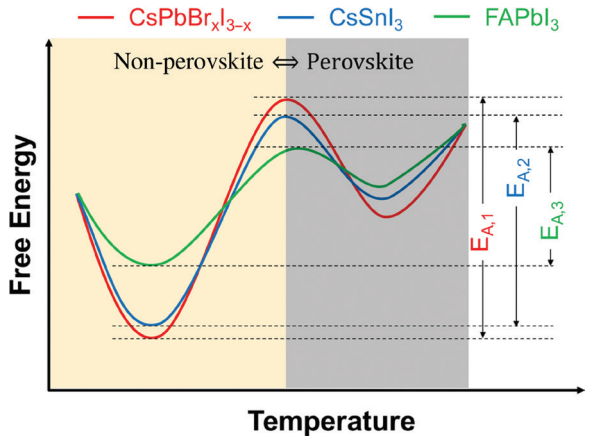

Figure 1. Schematic representation of an activation energy barrier for phase transition in typical halide perovskites.

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