Frontier Chemistry Center
フロンティア化学教育研究センター

講演会

The role of temperature in solid-state ceramic synthesis

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日 時：2022 年 12 月 20 日（火）16:30~17:30

場 所：工学部材料化学系棟 大会議室 MC526

要 旨：An emerging goal in the ab initio materials design community is to predict efficient synthesis recipes to functional oxide materials. Temperature plays a crucial role in solid-state synthesis, but it is difficult to predict which temperature is best to carry out a solid-state reaction, as it is difficult to distinguish whether temperature is playing a thermodynamic or kinetic role in a given solid-state reaction. Here, I will show that the phase evolution kinetics in solid-state synthesis can largely be anticipated from reaction enthalpies alone, meaning that we can qualitatively guide synthesis planning without the need for temperature-dependent free-energy calculations. However, recent in-situ XRD observations reveal a critical onset temperature for when a solid-state reaction initiates, which cannot be anticipated from any existing textbook theories. We derive a new explanation for this critical onset temperature from the liquidus curve of the phase diagram, showing that it corresponds to the metastable eutectic temperature. This provides guidance for what temperatures solid-state chemists should target the preparation of novel materials.

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