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

講演会

演 題：**Role of Structural Disorder in Influencing the Thermal Conductivity of Sulvanite-Related Compounds**

講 師：**Prof. Partha Pratim Jana**
IIT Kharagpur

日 時：2026 年 6 月 11 日（木）16:30～17:30

場 所：工学部 材料・化学系棟 2F MC213

主 催：北海道大学大学院総合化学院

共 催：北海道大学大学院工学研究院 フロンティア化学教育研究センター

要 旨：Low thermal conductive semiconductors have attracted huge attention for waste heat harvesting applications. Although the weak chemical bonding in the Cu/Ag-based chalcogenides is promising in suppressing heat transport, their ternary and quaternary analogues remain less explored. In this regard, the crystal structure and thermal conductivity of various Cu/Ag-containing sulvanite-type compounds are the focus of our ongoing investigation. In our recent study, we carried out both experimentally and theoretically analyses of the crystal structure, phase transition, and temperature-dependent lattice thermal conductivity (κ_L) of ACu_3TiQ_4 (A = Cu, Ag; Q = S, Se, Te).[1-6] The cubic crystal structures (space group $P\bar{4}3m$) of ACu_3TiQ_4 (A = Cu, Ag; Q = S, Se) are structurally similar to mineral sulvanite (Cu_3VSe_4), where a positionally disordered *A*-sites is located inside the sulvanite cage. Upon cooling, the symmetry reduction from cubic to a rhombohedral (space group $R3m$) structure occurs which is attributed to the partial ordering of the positionally disordered *A*- atoms. Interestingly, the lattice thermal conductivity of these compounds remains exceptionally low, varying in the range of ~0.2–0.7 W m^{-1} K^{-1} at room temperature. Density Functional Theory (DFT) calculations show that the presence of antibonding states of Cu(3*d*)/Ag(4*d*) −Q(4*p*) near the Fermi level (E_F) provides softness to the lattice framework. In addition, the positionally disordered sites play a crucial role in further softening the framework and provides large lattice anharmonicity. The low-lying optical phonon modes are mainly driven by the presence of soft lattice framework, positional disorder and associated rattling-like vibrations of Ag/Cu atoms. Their strong interaction with the heat-carrying acoustic phonon modes are key ingredients that explain the ultra- low lattice thermal conductivity.

References:
(1) ***Angew. Chem.*** **2021**, ***9188***, 9188-9195.
(2) ***Eur. J. Inorg. Chem.*** **2021**, ***2021,*** 5052-5059.
(3) ***Eur. J. Inorg. Chem.*** **2023**, ***26***, e202300219.
(4) ***Inorg. Chem.*** **2023**, ***62,*** 748–755.
(5) ***Chem. Mater.*** **2024**, ***36***, 5741–5752.
(6) ***Chem. Mater.*** **2024**, ***36***, 10773–10785.

連絡先：工学研究院応用化学部門 三浦 章（内線：7116）

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