

SEMINAR

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Understanding interface structure and evolution: Insights from ZnO and TiO₂

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Interfaces play a crucial role in determining the functional properties of materials. While modern high-resolution TEM and density functional theory enable atomic-scale characterization of interface structures and prediction of their stability, the atomistic mechanisms by which these structures form and evolve toward their stable configurations remain largely unresolved. In this lecture, I will show the process of water dissociation at the rutile (TiO₂)-water interface, which is triggered by a specific interface configuration, and how specific dopants induce domain inversion in ZnO via a cascade of solid-state atomic interactions. These two examples demonstrate how the combination of experimental and theoretical approaches allows us to go beyond the description of static structures towards their formation mechanisms, providing important insights into controlling interface formation and stability.

Kindly invited.