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ABSTRACT:

Exploring Grain Boundary Properties in Energy Materials Via Correlative Microscopy

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This invited talk explores the impact of grain boundary structures and compositions on the functional properties of various materials for photovoltaics, batteries, and other energy-related applications [1]. Examples of correlative microscopy studies highlight the potential to discover structure-property relationships at grain boundaries, essential for the design of energy devices to achieve superior performance [2].

A key focus will be on transport phenomena at grain boundaries, including mass, thermal, electrical, and ionic transport mechanisms. These transport phenomena are directly correlated with the charge defects that lead to a buildup of electric charges and potential barriers at the grain boundaries. In addition, applied electric fields can also induce boundary transitions that can affect grain boundary transport and other properties [3]. Finally, we demonstrate that these potential barrier heights can be tuned by modulating the chemical composition, structure, and carrier concentration of the grain boundaries.

Bibliography:

- [1] Structure and composition of grain boundaries and their impact on functional properties of energy materials, MRS Bulletin, 2026, accepted, in proof.
- [2] [1] O. Cojocaru-Mirédin and A. Devaraj, "Correlative microscopy and techniques with atom probe tomography: Opportunities in materials science," MRS Bull., vol. 47, no. 7, pp. 680–687, 2022, doi: 10.1557/s43577-022-00369-4.

[3] R. Wu, Y. Yu, S. Jia, C. Zhou, O. Cojocaru-Mirédin, and M. Wuttig, "Strong charge carrier scattering at grain boundaries of PbTe caused by the collapse of metavalent bonding," *Nat. Commun.*, vol. 14, no. 1, p. 719, 2023, doi: 10.1038/s41467-023-36415-1.