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Nanoscale Surface Chemistry for Perovskite Photovoltaics

Interfaces in semiconductor devices often contain high defect densities that affect carrier dynamics and long-term stability. In halide perovskites, probing these effects is particularly challenging due to their ionic lattices and complex interactions with adjacent materials. Although interface passivation is widely adopted, establishing direct correlations between interfacial structure and device performance remains a major challenge.

In this talk, I first present our work of structure-property relationship in Dion–Jacobson (DJ) perovskites, a promising class of stable photovoltaic absorbers. Using a non-destructive peel-off technique combined with spectroscopy and microscopy, we directly probe buried interfaces and reveal that multiscale inhomogeneities, more prevalent at buried layers than surfaces, act as performance-limiting defects. A sulfate-based inner-sphere complexation strategy is developed to passivate crystal terminations and promotes uniform crystal growth, yielding record efficiencies in DJ perovskite photovoltaics. I also share our recent findings that carrier-selective interface degradation is a key barrier to commercializing perovskite photovoltaics. In situ electrical tracking identifies fill-factor loss as a dominant degradation mode, linked to thermally induced disorder in commonly used molecular contacts. We address this by introducing Schiff-base cross-linking to stabilize these interfaces, resulting in significantly improved thermal and operational device stability.