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Theory and modeling of correlated ionic motions in hybrid organic-inorganic perovskites¹

ANDREW RAPPE, University of Pennsylvania

The perovskite crystal structure hosts a wealth of intriguing properties, and the renaissance of interest in halide (and hybrid organic-inorganic) perovskites (HOIPs) has further broadened the palette of exciting physical phenomena. Breakthroughs in HOIP synthesis, characterization, and solar cell design have led to remarkable increases in reported photovoltaic efficiency. However, the observed long carrier lifetime and PV performance have eluded comprehensive physical justification. The hybrid perovskites serve as an enigmatic crossroads of physics. Concepts from crystalline band theory, molecular physics, liquids, and phase transitions have been applied with some success, but the observations of HOIPs make it clear that none of these conceptual frameworks completely fits. In this talk, recent theoretical progress in understanding HOIPs will be reviewed and integrated with experimental findings. The large amplitude motions of HOIPs will be highlighted, including ionic diffusion, anharmonic phonons, and dynamic incipient order on various length and time scales. The intricate relationships between correlated structural fluctuations, polar order, and excited charge carrier dynamics will also be discussed.

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