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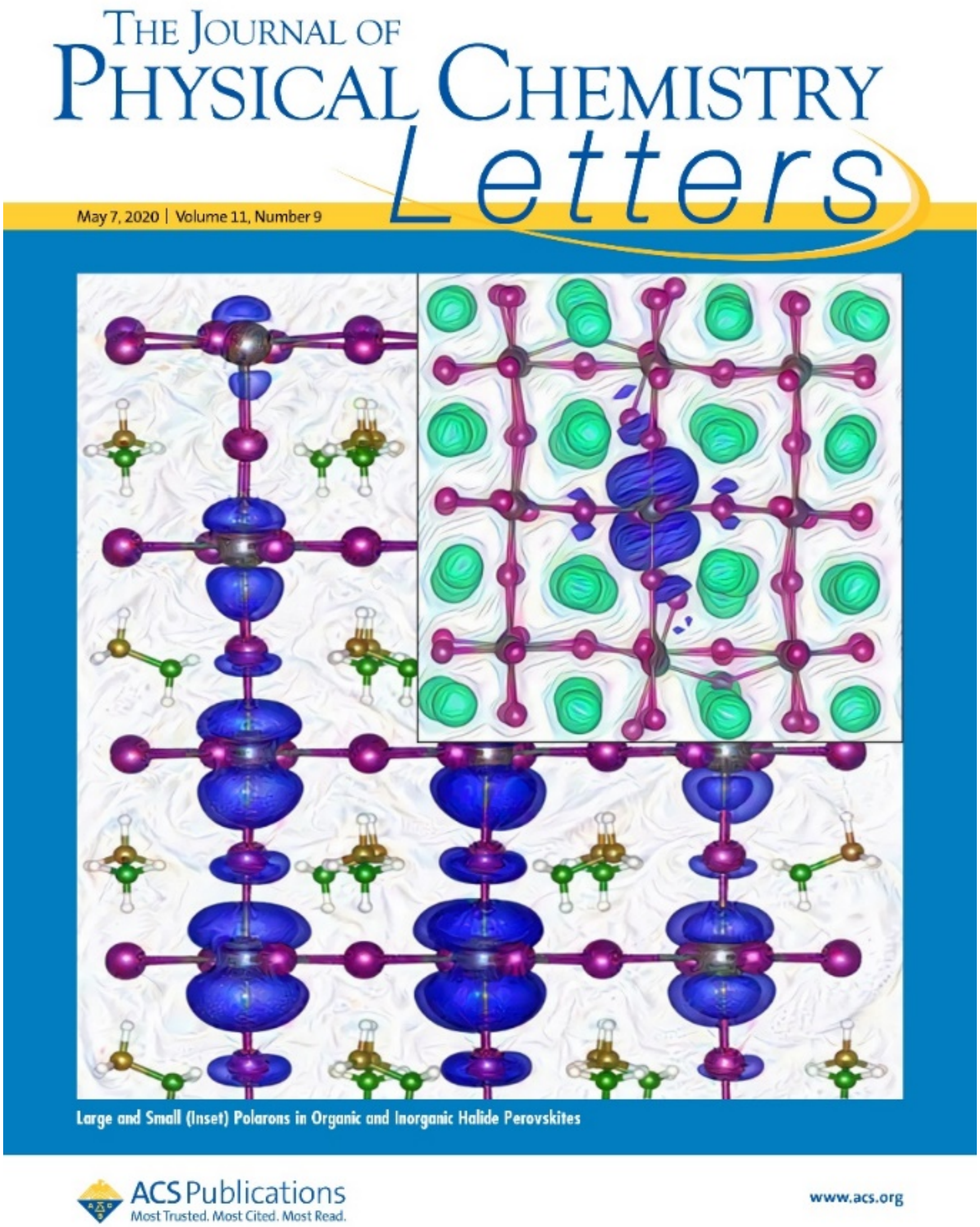
Is Polaron Formation Effective in Halide Perovskites?

Metal halide perovskites are emerging materials for a wide variety of next-generation optoelectronic devices from light-emitting diodes to solar cells to γ-ray detectors. The extraordinary photoactivity of these materials is often attributed to their unusually long charge-carrier recombination time. In a recently published Perspective, scientists in Los Alamos National Laboratory have summarized several extensively studied carrier transport mechanisms, such as electron−phonon scattering limited dynamics, ferroelectric effects, Rashba-type band splitting. The team particularly emphasizes on the possible formation of polarons that are the composite units of electronic charges and lattice-displacements. Highly polarizable lattices as well as short and long-range electron-phonon interactions form different types of polarons, screening the photo-generated charge carriers from the recombination processes.

The Perspective has been highlighted as the Cover Page of the publishing journal, The Journal of Physical Chemistry Letters, May 2020.



The Science

Metal halide perovskites (MHPs) have rapidly emerged as leading contenders in photovoltaic technology and other optoelectronic applications owing to their outstanding optoelectronic properties. After a decade of intense research, an in-depth understanding of the charge carrier transport in MHPs is still an active topic of debate. In this Perspective, authors discuss the current state of the field by summarizing the most extensively studied carrier transport mechanisms such as electron-phonon scattering limited dynamics, ferroelectric effects, Rashba-type band splitting, and polaronic transport. Ghosh et al. further extensively discuss the emerging experimental and computational evidence for dominant polaronic carrier dynamics in MHPs. Exploring both small and large polaron in MHPs, authors discuss their formation and effect on structural and carrier dynamics in these photoactive materials. Lattice distortion due to small polaron formation has been identified by recent Raman-spectroscopy based experimental work and predicted to be a probable reason for reversible photodegradation in these halide perovskites due to the formation of static charge pools. Detailed studies further suggest that compositional engineering, particularly controlled mixing of different sized A-cations, can partially mitigate the small polaron formation and enhance the stability of halide perovskites against degradation. Moreover, electron-phonon coupling in the ionic lattices of MHPs and dominant presence of long-range Coulomb potentials indicate the large polarons in these materials to be a dominant charge carrier. Such polaron formations can protect the photogenerated electrons and holes from recombination and defect-scattering, eventually providing long carrier lifetime and large diffusion length as found in MHPs. Finally, the authors outlined different physical and chemical approaches considered recently to study and exploit further the polaron transport in MHPs.

The Impact

The study elaborately discusses the charge carrier dynamics in halide perovskites, promising materials for next-generation optoelectronic devices. Due to the structural complexity and contradictory experimental and computational reports, the exact nature of carrier dynamics in these materials is a highly debated topic. The study summarizes most of the commonly believed transport mechanisms, providing the community an unbiased view of the current state of fundamental understanding on this topic. With great details of polaron formation and their transport in halide perovskites, the study emphasizes the dominance of such transport mechanisms. The Perspective will serve as a greatly valuable up-to-date report on the charge carrier dynamics in halide perovskites.

Research Details

The Perspective was written by Dibyajyoti Ghosh, Amanda Neukirch, and Sergei Tretiak in collaboration with Eric Welch and Alex Zakhidov from the Department of Physics, Texas State University, Texas.

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Publications

Polarons in Halide Perovskites: A Perspective, The Journal of Physical Chemistry Letters 11 (9), 3271-3286

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