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DOE BES FINAL TECHNICAL REPORT

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ABSTRACT

Hybrid metal halides, particularly main group halide perovskites, are a unique class of materials that offer exceptional optoelectronic properties along with a remarkable materials design space. Initial research on this class of materials was driven by the ability of the prototype hybrid 3D perovskite-structured compound methylammonium lead iodide to function as the active layer in thin film solar cells. It is now known that this class of materials comprise a large family with tunable band gaps, relatively high charge carrier mobilities in both single crystal and polycrystalline forms, and relatively low concentrations of (deleterious) electrically active states within the band gap. Beyond applications in solar cells, the potential of these materials has been extended to emitters in light emitting diodes, and active components of radiation detectors. Complementing new functionality, the design space for hybrid metal halides continues to increase with discovery of new structural motifs.

In this project, the combination of organic and inorganic functionalities has been employed to open pathways to the design and synthesis new, functional hybrid metal halides. Beyond the simple perovskites, Ruddlesden-Popper and Dion-Jacobsen compounds, and other variants, such as the newly advanced "hollow" perovskites have been studied. The materials have provided routes to understanding the unique electronic properties of hybrid metal halides because of their natural quantum well structures as well as other means of controlling band gaps and band dispersions. Understanding these materials, including the design rules for their formation, their structures and compositions in bulk and in thin films form, and the role of local (non-crystallographic) structure has an important aspect of this endeavor. The goal of advancing new materials and new fundamental understanding within this deceptively simple, yet fascinating class of compounds, so richly endowed with interesting and useful functionality, has been fulfilled.

EXECUTIVE SUMMARY

Hybrid metal halide perovskites based around main group elements are a unique class of materials that have offered exceptional optoelectronic properties along with a remarkable materials design space The initial study of this class of materials was driven by the performance of methylammonium (MA) lead iodide $CH_3NH_3PbI_3$, also referred to as $MAPbI_3$ in thin film solar cells. It is now known that $MAPbI_3$ and its alloys with other halides and *A*-site cations comprise a set of materials with tunable band gaps, relatively high charge carrier mobilities in both single crystal and polycrystalline forms, and relatively low concentrations of electrically active states within the band gap. The potential of these materials has been demonstrated in applications ranging from solar cells to light emitting diodes, to radiation detectors. The design space for hybrid metal halides has continued to expand with discovery of new structural motifs. The combination of organic and inorganic functionalities has opened pathways to design and to synthesize new hybrid metal halides. For example, Ruddlesden-Popper (RP) and Dion-Jacobsen (DJ) phases have provided a route to understand the unique electronic properties of metal halides because of their natural quantum well structures. Emerging materials, such as hollow perovskites, have challenged conventional rules of geometric tolerances for incorporation of organic species leading to optoelectronic behavior that is intermediate to 3D and 2D phases.

In this research context, already heavily contributed to by the PIs of this project, the following *questions* were addressed in the work that was proposed: (i) Can we design materials that bridge 3D and quantum confined optoelectronic behavior? (ii) How do we properly characterize materials that bridge nanoparticles and layered perovskites? (iii) How do misfitting organic cations impact structure, dimensionality, and property? (iv) What is the role of exposure to light in phase stability and structure? (v) How do the relatively soft lattices of hybrid metal halides respond to mechanical strain and how can strain be used to control their physical properties? (vi) How does going beyond Pb^{2+} and neighboring central ions to transition elements enhance functionality?

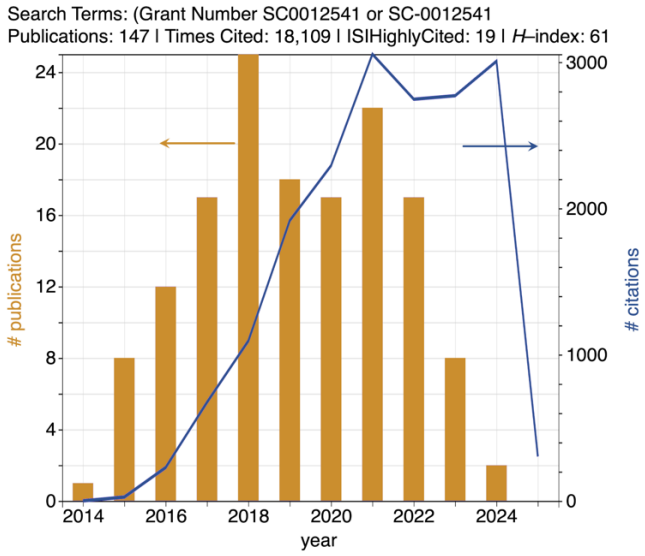

Figure 1. Results of a Web of Science analysis of archival journal publications arising from this project (data downloaded late February 2025).

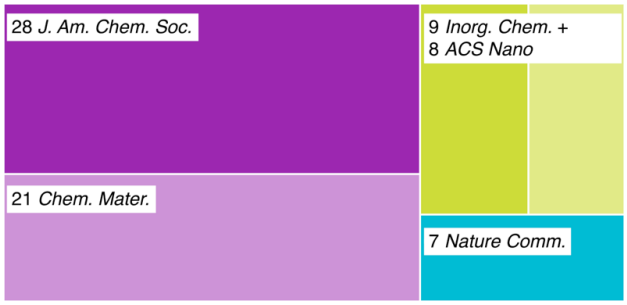

Figure 2. Graphical representation of the top 5 journals in which publications acknowledging SC-0012541 have appeared.

The anticipated *goals and outcomes* of what was proposed included to: (i) Expand synthesis and chemistry to expand the hybrid halide materials research domain. (ii) Develop a portfolio of materials which display the greater stability of 2D metal halides with the desired electronic performance of 3D perovskites. (iii) Help to advance control of functional metal halides by understanding the growth processes and performance in polycrystalline films. (vi) Probe new functionality based on transition metal centers. (v) Synergistically employ electronic structure theory to understand structural and functional behavior. It was believed that addressing the questions posed through the systematic development of the proposed goals would result in the following: (i) An ability to carefully control chemistry and structure in these materials. (ii) The ability to develop new materials for lighting and other optoelectronic applications. (iii) The ability to develop new classes of hybrid magnetic halides.

The collaboration project has been highly productive and impactful. In terms of public cations, this is captured in the Web of Science results presented in **figure 1**. As many as 147 archival journal publications acknowledge this project as obtained from a Web-of-Science search performed end-February 2025. Approximately between half and two-thirds of these articles are solely due to this project with the remaining emerging from collaborations, often though the sharing of the unique samples developed within this collaboration.

The articles have been published in reputable journals; for example, 28 of the articles are in the *Journal of the American Chemical Society*, the large majority of which were led by graduate students or postdoctoral researchers supported by the project (**figure 2**). In terms of training personnel, the project has involved exceptional early career researchers some of whom are already establishing strong, independent careers in academia, industry, or National Labs. Others are well on their way to doing so. The project has had the good fortune to leverage several fellowship-holding graduate students and self-funded postdoctoral researchers, which allowing more early career researchers to be involved in the work than would otherwise have been possible.

While it is impractical in a brief report to summarize all the accomplishments of this project, some key recent accomplishments are presented here. The exemplary studies presented here are representative of the questions addressed and they closely hew to the anticipated goals and outcomes that were originally proposed.

DESCRIPTION OF SELECT OUTCOMES (FOCUS ON THE LAST THREE YEARS OF THE PROJECT)

Layered Hybrid Lead Iodides with Short Interlayer Distances [1]: Layered hybrid perovskites comprise modular components that are individually highly tunable, resulting in materials with a range of structures and properties. In these layered materials, the usual assumption is of two-dimensional electronic behavior, because of the relatively large separations between the inorganic layers. Within this collaboration, two layered, hybrid lead iodide perovskites have been reported that possess unusually short interlayer distances: $(IPA)_2(MA)Pb_2I_7$ and $(ACA)(MA)PbI_4$ (IPA = isopropylammonium, MA = methylammonium, ACA = acetamidinium). These compounds, prepared from mixing small organic cations, crystallize in a Ruddlesden–Popper type structure, or in a previously reported (by some of us) structure type with alternating cations in the interlayer space, respectively. The crystal structures of these compounds were established and have been compared in detail with related structures, with the electronic structures analyzed using density functional theory-based calculations suggesting significant dispersion even between the layers, due to the short non-bonded contacts between the iodides (figure 3). Time-resolved microwave conductivity measurements were employed to provide insight into charge transport in these compounds. This work has helped bridge the world of 3D halide perovskites with the world of the more usual 2D Ruddlesden–Popper or Dion-Jacobsen compounds whose electronic structures show little or no dispersion perpendicular to the inorganic slabs.

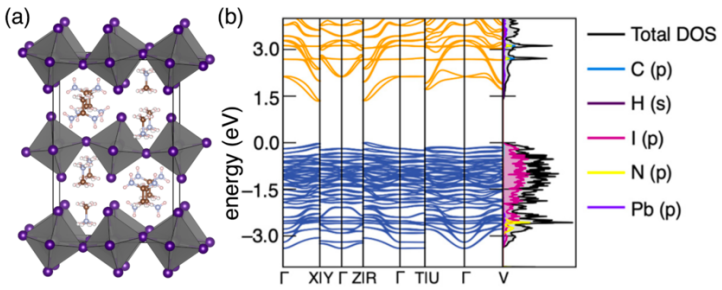

Figure 3. Crystal structure of (ACA)(MA)PbI4 with very short non-bonded contacts between the I^- in the perovskite layers. (b) Band structure displaying significant band dispersion (covalency) from inter-slab hopping.

Defect Emission from "Hollow" Perovskites [2]: The prototypical hybrid halide perovskites APbX_3 suffer from poor stability under ambient conditions of light, oxygen, and moisture. It was shown within this collaborative effort that when ethylenediamine is one of the amines incorporated into the preparation of the 3D hybrid halide perovskites, so-called "hollow" perovskites emerge, with greatly enhanced stability to the ambient atmosphere and to light. In these materials, some of the extra-large organic cation (or di-cation) extends itself beyond the usual A site in the unit cell, to result in vacant M = Sn or Pb sites, and hence the term "hollow". During this project, a new family of 3D highly defective yet crystalline "hollow" bromide perovskites with general formula $(FA)_{1-x}(en)_xPb_{1-0.7x}Br_{3-0.4x}$ where FA = formamidinium, en = ethylenediammonium, x ranging from 0.00 to 0.42 were prepared and characterized using a plethora of techniques. Pair distribution function analysis of synchrotron X-ray scattering shed light on the local structural coherence, revealing a wide distribution of Pb–Pb distances in the crystal structure because of the Pb/Br-deficient nature and en inclusion. A depiction of the structure that is consistent with NMR and PDF studies is displayed in **figure 4**. By manipulating the number of Pb/Br vacancies, it was possible to finely tune the optical properties resulting in blue shifting the band gap from 2.20 eV all the way to 2.60 eV for the $x = 0.42$ sample. An unexpected outcome was that at $x > 0.33$, the material exhibited strong broad light emission with 1 % photoluminescence quantum yield (PLQY) that was maintained after exposure to air for more than a year. This is the first example of strong broad light emission from a 3D hybrid halide perovskite, demonstrating that judicious defect engineering is an excellent tool for customizing the optical properties of these semiconductors. This work also demonstrates the defect tolerant nature of engineered hybrid halide perovskites, making these materials appropriate for use in applications such as hard radiation resilience. Other contributions on ``hollow'' perovskites that have emerged during this reporting period include work on ion transport in these materials and a contribution on their thermochemistry where it has been suggested that they are entropy stabilized.

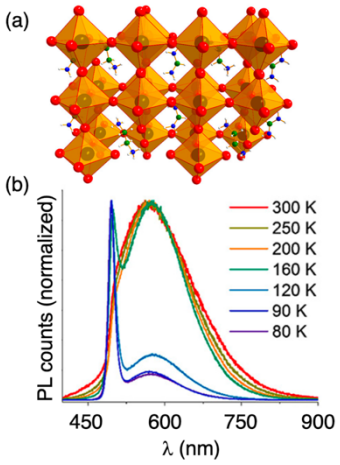

Figure 4. (a) Schematic depiction of the local and average structure of "hollow" $(FA)_{1-x}(en)_xPb_{1-0.7x}Br_{3-0.4x}$ consistent with a range of structural probes, and (b) luminescence as a function of temperature of a "hollow" lead bromide perovskite.

Halide Perovskites and Variants with Transition Metals [3]: During the most recent renewal of this project, a proposed area of research was the expansion of the portfolio of materials to develop new compounds containing transition metals, including open shell (*i.e.*, magnetic) 4d and 5d transition metals. Within this research domain, inorganic and hybrid double perovskites with Ru^{3+} and vacancy-ordered double perovskites with Ru^{4+} have been prepared and characterized, including their structure, optical, and magnetic properties. A new class of compounds for these metals: layered double perovskites have also been prepared. Hybrid layered double perovskite halides comprise hexa-coordinated 1+ and 3+ metals in the octahedral sites within perovskite layers and organic amine cations between the layers. Progress on such materials had hitherto been limited to compounds containing main group 3+ ions isoelectronic with Pb^{2+} (such as Sb^{3+}

and Bi^{3+}). During this past reporting period eight HLDP halides from the $A_2M^{I}M^{III}X_8$ family, where A = paraphenylenediammonium (PPDA), 1,4-butanediammonium (1,4-BDA), or 1,3-propanediammonium (1,3-PDA); M^{I} = Cu or Ag; M^{III} = Ru or Mo; X = Cl or Br have been prepared and characterized. **Figure 5** shows a scheme of some of the new compounds prepared and characterized. The optical band gaps, which lie in the range 1.55 eV to 2.05 eV, are tunable according to the layer composition, but are largely independent of the spacer. Magnetic measurements carried out for $(PPDA)_2AgRuCl_8$ and $(PPDA)_2AgMoCl_8$ showed no obvious evidence of a magnetic ordering transition. The layered double perovskite structure is perhaps more widespread, particularly when oxides are considered, than has hitherto been appreciated and a recent review from some of the team has emphasized this point.

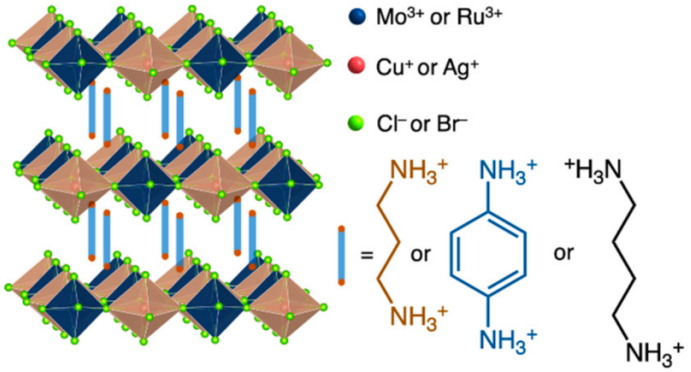

Figure 5. Exemplary Dion-Jacobsen type hybrid layered double perovskite compounds prepared and studied here. The study also encompassed Ruddlesden-Popper variants.

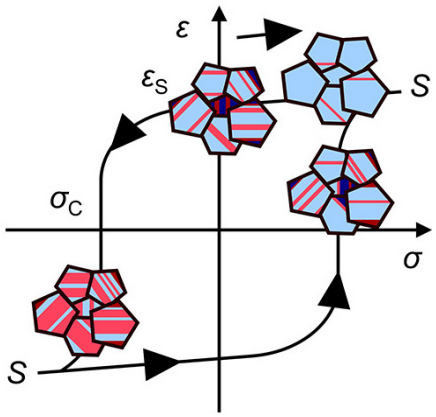

Figure 6. Straining thin films of $MAPbI_3$ deposited on flexible substrates results in the formation of twin domains due to the ferroelastic nature of the material, indicated schematically on the right.

Ferroelastic Behavior in Films [4]: While thin films of active materials are required for device behavior, it has now been widely appreciated that growing films of hybrid halide perovskites can be challenging, including retaining the composition of bulk crystals, and additionally, new aspects of behavior can be observed in thin films. For example, mechanical strain can modify the structural and electronic properties of methylammonium lead iodide $MAPbI_3$. The consequences of ferroelastic hysteresis, which involves the retention of structural memory upon cycles of deformation, have been studied here for polycrystalline thin films of $MAPbI_3$. Repeatedly bent films were examined using grazing incidence wide-angle X-ray scattering to quantitatively characterize the strains and proportions of twin domains as seen in **figure 6.** Approximate locations for the coercive stress and saturation on the ferroelastic stress–strain curve have been identified, and changes to the stress–strain curve with cyclic strain are characterized. The presence of specific twin domains is found to correlate to previously reported strain and defect heterogeneity in $MAPbI_3$ films. Domains from differently strained twin sets interact with each other. Long-term stability testing reveals that the domain walls are highly immobile over extended periods. Nucleation of new domain walls occurs for specific mechanical strains and correlates closely with degradation. The results help to explain the behavior of ion migration, degradation rate, and photoluminescence in thin films under compressive and tensile strain.

Hybrid Perovskite Synthesis from Solution: Layered or Nano? [5]: Controlling the structure of layered hybrid metal halide perovskites, such as the Ruddlesden–Popper (R-P) phases, is challenging because of their tendency to form mixtures of varying composition. Colloidal growth techniques, such as anti-solvent precipitation, form dispersions with properties that match bulk layered R-P phases, but controlling the composition of these particles remains an open problem. The microstructure of particles of R-P phases of methylammonium lead iodide prepared by anti-solvent precipitation from ternary mixtures of alkylammonium cations have been studied using a range of techniques. In these systems, one cation can form perovskite phases ($CH_3NH_3^+$) and the other two promote layered structures as spacers (*e.g.*, $C_4H_9NH_3^+$ and $C_{12}H_{25}NH_3^+$). It has been found that the alkylammonium spacers pack with constant methylene density in the R-P interlayer and exclude interlayer solvent in dispersed colloids, regardless of length or branching. Using this result, the competition between cations that act as spacers between layers, or as grain-terminating ligands, are demonstrated to determine the colloidal microstructure of layered R-P crystallites in solution. Optical measurements reveal that quantum well dimensions can be tuned by engineering the ternary cation composition.

Transmission synchrotron wide-angle X-ray scattering and small-angle neutron scattering (**figure 7**) reveal changes in the structure of colloids in solvent and after deposition into thin films. Specifically, spacers are found to alloy between R-P layers if they share common steric arrangements but tend to segregate into polydisperse R-P phases if they do not mix. The structure of colloidal 2D perovskites appears to be determined by a sensitive balance between spacer–spacer and spacer–solvent interactions, and future synthetic progress for solution-processed 2D perovskites requires a careful accounting of these phenomena. More generally, the interlayer region of layered 2D perovskites is responsive to solvent-mediated mixing behavior among different insulating cations. These results suggest that the molecular design of spacer cations and solution processing techniques can be used to engineer the growth of layered perovskites.

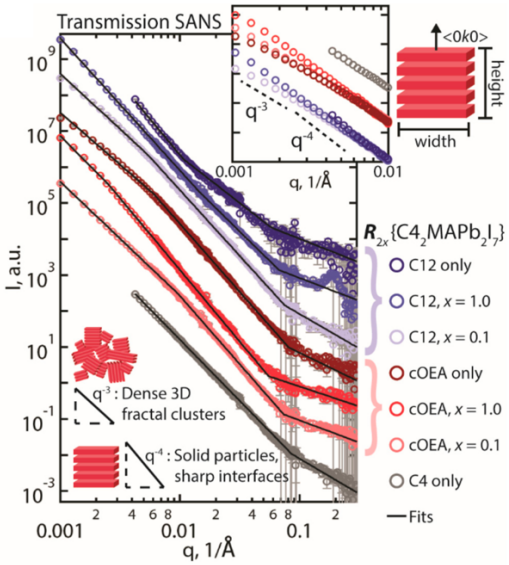

Figure 7. Small-angle neutron scattering patterns from colloidal dispersions in deuterated toluene prepared with different precursors and ligands. The inset shows the low–*q* region of the same data.

On the Role of Lone Pairs in Hybrid Halide Perovskites [6,7]: The presence of ns^2 lone pair electrons on divalent Sn ($n = 5$) and Pb ($n = 6$) when these cations occupy the M site in all-inorganic and hybrid halide AMX_3 perovskites distinguishes these materials from the familiar semiconductors such as the diamondoid (zinc blende, wurtzite, chalcopyrite, …) semiconductors traditionally employed in optoelectronics. However, their role in the perovskites has not been unambiguously established. These electrons are stereochemically active, albeit often in a hidden fashion, resulting in unusual and highly anharmonic lattice dynamics that are linked to many of the special optoelectronic properties displayed by this material class. Some lone pair containing

molecular and extended structures from the perspective are displayed in **figure 8**. In a perspective article published during this collaboration, the connections between this atypical electronic configuration and the electronic structure and lattice dynamics of compounds have been examined. The lone pair can potentially lead to favorable bandwidths and band alignments, mobile holes, large ionic dielectric response, large positive thermal expansion, and even possibly defect-tolerant electronic transport. Taken together, the evidence suggests that other high-performing semiconductors may be found among compounds with lone pair-bearing cations in high symmetry environments and a high degree of connectivity between atoms.

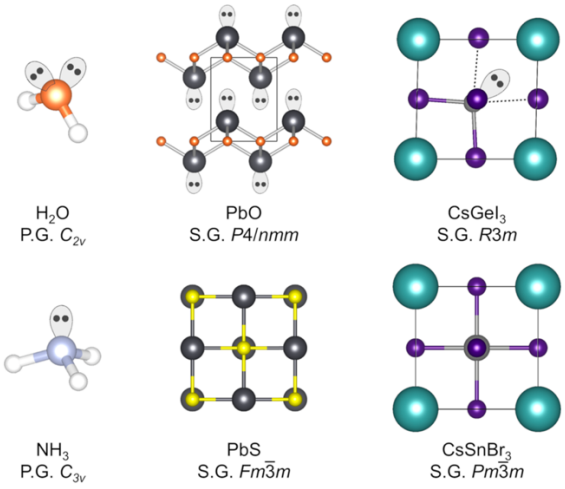

Figure 8. Molecular and crystal structures of water, ammonia, litharge PbO, rock-salt PbS, and perovskites $CsGeI_3$ and $CsSnBr_3$ (both at room temperature). Note that lone pairs in PbS and $CsSnBr_3$ are obscured by the symmetrical coordination polyhedra.

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