

Lausanne talk – May 9 – 16:15-17:15 – CE 14

Amazing 3D and 2D Halide Perovskites: All the things they do

Sion talk – May 10 – 10:30-11:30 – Zeuzier Room

1D, 2D, 3D Perovskites and perovskitoids: structure diversity and applications

Mercouri G. Kanatzidis

Department of Chemistry, Northwestern University, Evanston, IL 60208, USA.

Abstract :

Three-(3D) and two-dimensional (2D) layered halide perovskites are highly promising semiconductors for optoelectronic applications ranging from solar cells, light emitting diodes, soft radiation detector, hard radiation detectors, etc. The 3D versions of these compounds adopt the three-dimensional ABX_3 perovskite structure, which consists of a network of corner-sharing BX_6 octahedra, where the B atom is a divalent metal cation (typically Ge^{2+} , Sn^{2+} or Pb^{2+}) and X is a monovalent anion (typically Cl^- , Br^- , I^-); the A cation is selected to balance the total charge and it can be a Cs^+ or a small molecular species. Another class of materials gaining significance are the two-dimensional (2D) perovskites -a blend of perovskites with layered crystal structure- (Ruddlesden-Popper type) offer a greater synthetic versatility and allow for more specialized device implementation due to the directional nature of the crystal structure. A remarkable advantage of the 2D perovskites is the readily tunable functionality by incorporating a wide array of organic cations into the 2D framework and by controlling the slab thickness, in contrast to the 3D analogues which have limited scope for structural engineering. We present the new homologous series, $(C(NH_2)_3)(CH_3NH_3)_nPb_nI_{3n+1}$ ($n = 1, 2, 3$), of layered 2D perovskites which is different from Ruddlesden-Popper type. These compounds adopt an unprecedented structure type which is stabilized by the alternating ordering of the guanidinium and methylammonium cations in the interlayer space (ACI). The these 2D perovskites combine structural characteristics from both Dion-Jacobson (DJ) and Ruddlesden-Popper (RP) structure archetypes. We also report the first examples of hybrid DJ hybrid 2D lead iodide perovskites which consist of thick perovskite slabs ($n > 1$) with layer number (n) ranging from 1 to 5. We describe two new DJ perovskite series based on bivalent (+2) spacer cations deriving from a piperidinium (C_5NH_{12}) organic backbone. The new DJ perovskites are built from 3AMP (3AMP = 3-(aminomethyl)piperidinium) and 4AMP (4AMP = 4-(aminomethyl)piperidinium) spacers and methylammonium (MA) perovskitizers cations to form $A'(MA)_{n-1}Pb_nI_{3n+1}$ ($A' = 3AMP$ or $4AMP$, $n = 1-4$) homologous series acting as spacers. Surprisingly, a slight difference in the position of the $-CH_2NH_3^+$ group on the piperidine chair (3- and 4- position with respect to the piperidine nitrogen) exerts a strong influence on the crystal structure, which is reflected on the distortion of the inorganic layers. This difference has a major impact on the optical and electronic properties.

Biography :

Mercouri G. Kanatzidis obtained a B.Sc. degree from Aristotle University in Greece and received his Ph.D. degree in chemistry from the University of Iowa in 1984. He was a postdoctoral fellow at the University of Michigan and Northwestern University from 1985 to 1987 and is currently the Charles E. and Emma H. Morrison Professor of Chemistry at Northwestern University. He also holds an appointment at Argonne National Laboratory. Professor Kanatzidis is a AAAS and MRS fellow and has received numerous awards including the most recent ACS Award for Inorganic Chemistry and ENI Award for Renewable Energy.