

Presents

Lone Pairs in the Halide Perovskites, Hidden or Otherwise

by Prof Ram Seshadri

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Abstract

The ABX_3 halide perovskites that have attracted so much renewed attention mostly possess $B = \text{Sn}^{2+}$ or Pb^{2+} , with ns^2 lone pairs of electrons. These lone pairs are frequently hidden, in the sense that the crystal structures are not consistent with the presence of a stereochemically active lone pair, that would for example, result in certain characteristic distortions of BX_6 polyhedra in the structure. Such hidden lone pairs can be seen in many of the perovskites including the hybrids with methylammonium [$A = \text{CH}_3\text{NH}_3^+$] and formamidinium [$A = \text{CH}(\text{NH}_2)_2^+$], where the lone pairs are associated with proximal instabilities that can profoundly influence materials properties. We will discuss the understanding that we have developed from extensive real and k -space studies of local and average structure in these materials using synchrotron and neutron scattering. DFT calculations and NMR studies complement the structural studies to obtain a coherent picture of what is happening, and where all the red herrings are.

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Speaker



Ram Seshadri is the Fred and Linda R. Wudl Professor of Materials Science at UC Santa Barbara, in the Materials Department and the Department of Chemistry and Biochemistry. He received his PhD in Solid State Chemistry in 1995 from the Indian Institute of Science, Bangalore, and after some years as a postdoctoral fellow in Europe, returned to Bangalore as an Assistant Professor in 1999. He moved to UC Santa Barbara in 2002, where he has been Professor since 2008. At UCSB, he also serves as the Director of the Materials Research Laboratory: A National Science Foundation Materials Research Science and Engineering Center (NSF-MRSEC). His research — embodied in 330+ publications — addresses the topic of structure-property relations in crystalline inorganic materials, with a focus on materials for energy applications. He is a Fellow of the Royal Society of Chemistry, the American Physical Society, and the American Association for the Advancement of Science. He serves as the Associate Editor of *Annual Reviews of Materials Research* (on the Committee since 2008), and as an Associate Editor of *Chemistry of Materials* (since 2015).

ALL ARE WELCOME!

Host: Prof John Wang