**化学学科前沿-无机固体功能材料学术报告**

**Impact of Local Structure on Transparent Conductors**

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**Hybrid Halide Perovskites and Related Materials: Contraindicated Optoelectronic Materials**

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地点：南开大学元素所合成楼二楼报告厅

欢迎参加

化学学院先进能源材料化学教育部重点实验室

**Impact of Local Structure on Transparent Conductors**

The integrated process of addressing functionality and stability followed by laboratory synthesis and characterization could be expanded to more complex systems, such as the anion-deficient, fluorite related family that is particularly prominent in transparent conductors (TCs).1 For example, Zn0.456In1.084Ge0.460O3 (ZIGO) adopts a never before observed fluorite and bixbyite related structure.2 The possible anion deficiencies of fluorite produce a complex cation topological network, with varied local structures whose impact on TC properties is not well understood. Indeed, thus far, in fluorite-based materials only 6-coordinate cation sites have received any widespread attention in the TC field. We have taken the first steps in investigating the impact of alternative local structures on TC properties. Our initial investigations utilize Ga3-xIn5+xSn2O16 (0.3 ≤ x ≤ 1.6), which has its own complex local structures which span four differently coordinated sites.3-4 The combination of x-ray, neutron and electron diffraction studies has allowed a deeper understanding of the optimal experimental synthetic conditions and properties.

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(2) Rickert, K.; Sedefoglu, N.; Malo, S.; Caignaert, V.; Kavak, H.; Poeppelmeier, K. R. *Chem. Mater.*, **2015**, *27*, 5072-5079.

(3) Dolgonos, A.; Lam, K.; Poeppelmeier, K.R.; Freeman, A.J.; Mason, T.O. *J. Appl. Phys.*, **2014**, *115*, 013703.

(4) Rickert, K.; Huq, A.; Lapidus, S.H.; Wustrow, A.; Ellis, D.E.; Poeppelmeier, K.R. *Chem. Mater.*, **2015**, *27*, 8084-8093.



Kenneth R. Poeppelmeier，美国西北大学化学系教授，超导科学与技术中心副主任，曾兼任美国化学会无机化学-固体化学委员会主席，在1993-2013年期间担任Inorganic Chemistry副主编，目前是Chemistry of Materials、Journal of Alloys and Compounds、CHEMtracks、Solid State Sciences等重要学术期刊的编委。他在无机化学、材料化学、能源化学等领域开展研究工作，目前的主要研究兴趣是无机固体新材料的探索合成、表征，以及其在催化、电池、透明导体和非线性光学材料等领域的应用研究，是该领域享有很高知名度的专家，已在Science、Nature、Nature Chemistry、 Nature Materials、 J. Am. Chem. Soc.等学术刊物上发表论文200余篇。

**Hybrid Halide Perovskites and Related Materials: Contraindicated Optoelectronic Materials**

The recent explosion of interest in the functionally and architecturally diverse perovskite-halide–derived materials has been due to their potential as PV absorbers and sensitizers. However, while important, these applications represent only a small part of what these materials are capable of. Recent studies have revealed several important knowledge gaps in our understanding of these systems and raised a number of fundamental questions with regard to the prospects for developing innovative new variants with enhanced properties. In particular, there is the recognition that these materials exhibit useful yet contraindicated properties, or properties that usually do not coexist in the same material. This talk will cover Bi-based alternatives to the standard Pb–I materials,[1,2]. Some subtle structure features and transitions at low temperatures in the standard materials,[3] that appear to impact properties,[4] will be described. Finally, the use of optoelectronically active cations to develop new systems and prospects for other novel systems will be discussed.[5]

1. A. J. Lehner, D. H. Fabini, H. A. Evans, C.-A. Hébert, S. R. Smock, J. Hu, H. Wang, J. W. Zwanziger, M. L. Chabinyc, and R. Seshadri, Crystal and electronic structures of complex bismuth iodides *A*3Bi2I9 (*A* = K, Rb, Cs) related to perovskite: Aiding the rational design of photovoltaics, *Chem. Mater.* **27** (2015) 7137–7148.
2. A. J. Lehner, H. Wang, D. H. Fabini, C. D. Liman, C.-A. Hébert, E. E. Perry, M. Wang, G. C. Bazan, M. L. Chabinyc, and R. Seshadri, Electronic structure and photovoltaic application of BiI3, *Appl. Phys. Lett.* **107** (2015**)** 131109.
3. D. H. Fabini, T. Hogan, H. A. Evans, C. C. Stoumpos, M. G. Kanatzidis, and R. Seshadri, Dielectric and thermodynamic signatures of low temperature glassy dynamics in the hybrid perovskites CH3NH3PbI3 and HC(NH2)2PbI3, *J. Phys. Chem. Lett.* **7** (2016) 376–381.
4. J. G. Labram, D. H. Fabini, E. E. Perry, A. J. Lehner, H Wang, A. M. Glaudell, G. Wu, H. Evans, D. Buck, R. Cotta, L. Echegoyen, F. Wudl, R. Seshadri, and M. L. Chabinyc, Temperature-dependent polarization in field-effect transport and photovoltaic measurements of methylammonium lead iodide, *J. Phys. Chem. Lett.* **6** (2015) 3565–3571.
5. H. Evans, A. Lehner, J. Labram, D. Fabini, O. Barreda, S. Smock, G. Wu, M. Chabinyc, R. Seshadri, and F. Wudl, (TTF)Pb2I5: A radical cation-stabilized hybrid lead iodide with synergistic optoelectronic signatures. *Chem. Mater.***28** (2016) 3607–3611.



Ram Seshadri received his PhD in Solid State Chemistry in 1995 from the Indian Institute of Science, Bangalore, and after some years as a post-doctoral fellow in Europe, returned to Bangalore as an Assistant Professor in 1999. He moved to UC Santa Barbara in 2002, and was promoted to the rank of Associate Professor with tenure in 2006. Since 2008, he has been a Professor in the Materials Department and the Department of Chemistry and Biochemistry. 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 work, embodied in over 280 publications, broadly 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, and of the American Physical Society. He has served on the Editorial Committee of Annual Reviews of Materials Research since 2008, and as an Associate Editor of Chemistry of Materials since 2015. He previously served as Associate Editor for the Journal of Materials Chemistry.