Poster

Structure-property relationships in oxide ion conductors for energy applications: insight from diffraction, total scattering and spectroscopy

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An in-depth understanding of the structure – property relationships is essential for the successful discovery and development of new functional materials capable of overcoming the limitations of the currently used ones. As the materials' complexity increases, characterisation using a range of scattering-based techniques and complementary methods, as well as state-of-the-art data analysis approaches and computational simulations, is essential in providing this insight.

This presentation will give an overview of our work on the development of oxide ion conductors, some of which are the best-in-class performing materials. It will cover the elucidation of key design principles, defects and mechanisms giving rise to ionic mobility; the development and use of advanced structural data analysis methodologies capable of tackling exceptionally complex crystallographic problems arising from phase transitions; the complementary use of long-range and local structural probes in understanding the structure, disorder and properties. In addition, it will illustrate the understanding of the oxide-ion dynamics in solid electrolytes which quasielastic neutron scattering, supported by ab-initio molecular dynamics calculations, can provide.

Examples will include ionic conductors belonging to several different structural families, such as fluorite [1, 6], apatite [3] and perovskite-related [2, 4, 5] materials.

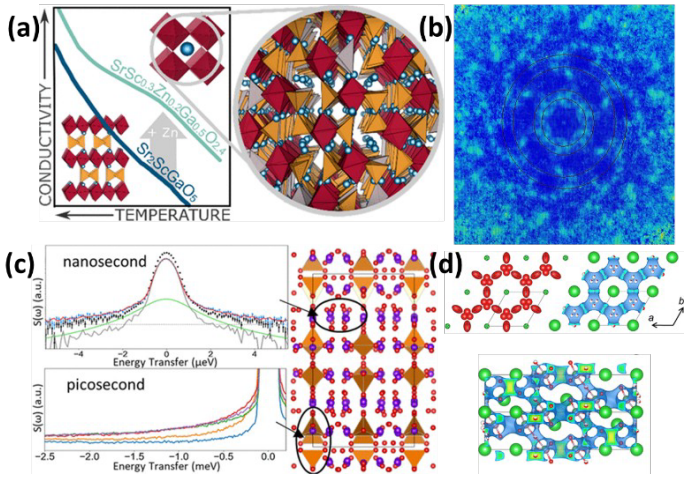

Figure 1. (a) Composition – structure – property relationships in oxygen-deficient perovskites. (b) Single crystal neutron diffuse scattering from a disordered apatite-type silicate. (c) QENS signatures of the oxide ion dynamics in a bismuth vanadate with fluorite- type superstructure. (d) Relationships between structure, atomic displacement parameters and facile ionic migration pathways in a hexagonal perovskite-related oxide ion conductor.

[1] Schwaighofer, B., Gonzalez, M. A., Appel, M., Koza, M. M & Evans, I. R. (2023). *Chem. Mater*., **35**, 3, 1125.

[2] Fuller, C. A., Murrell, J. I., Blom, D. A., Vogt, T., Zhang, W. Halasyamani, P. S., Evans, I. R. & Evans, J. S. O. (2022). *Chem. Mater*., **34,** 7, 3185.

[3] Fuller, C. A., Gutmann, M. J., Ling, C. D., Wang, C. H., Zhang, W. Halasyamani, P. S., Evans, I. R. & Evans, J. S. O. (2022). *J. Mat. Chem. A*, **10**, 27, 14576.

[4] Fuller, C. A., Blom, D. A., Vogt, T., Evans, I. R. & Evans, J. S. O. (2021). *J. Amer. Chem. Soc*., **144,** 1, 615.

[5] Auckett, J. E., Milton, K. L. & Evans, I. R. (2019). *Chem. Mater*., **31**, 5, 1715.

[6] Peet, J. R., Fuller, C. A., Frick, B., Koza, M. M., Johnson, M. R., Piovano, A. & Evans, I. R. (2019). *J. Amer. Chem. Soc*., **141,** 25, 9989.