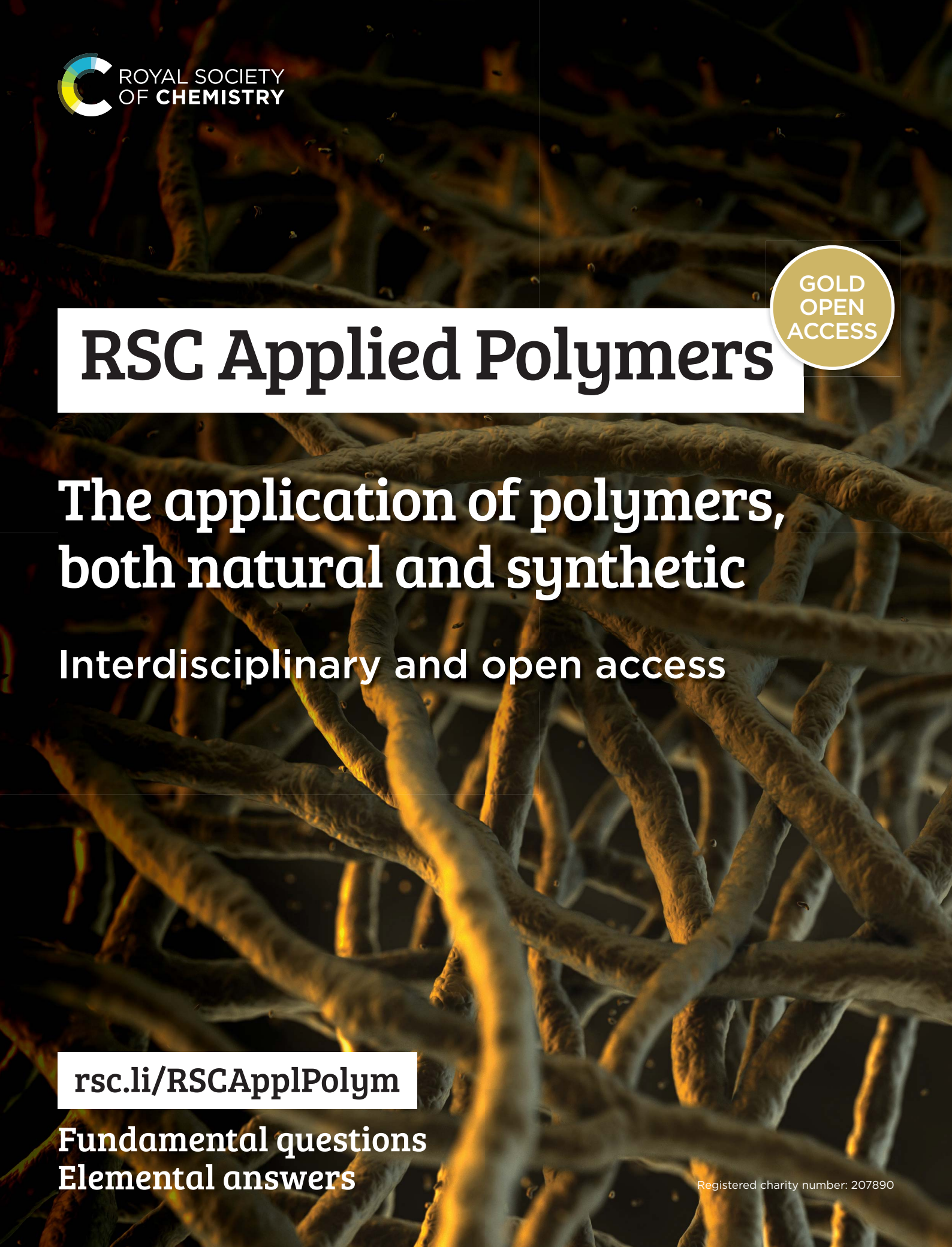
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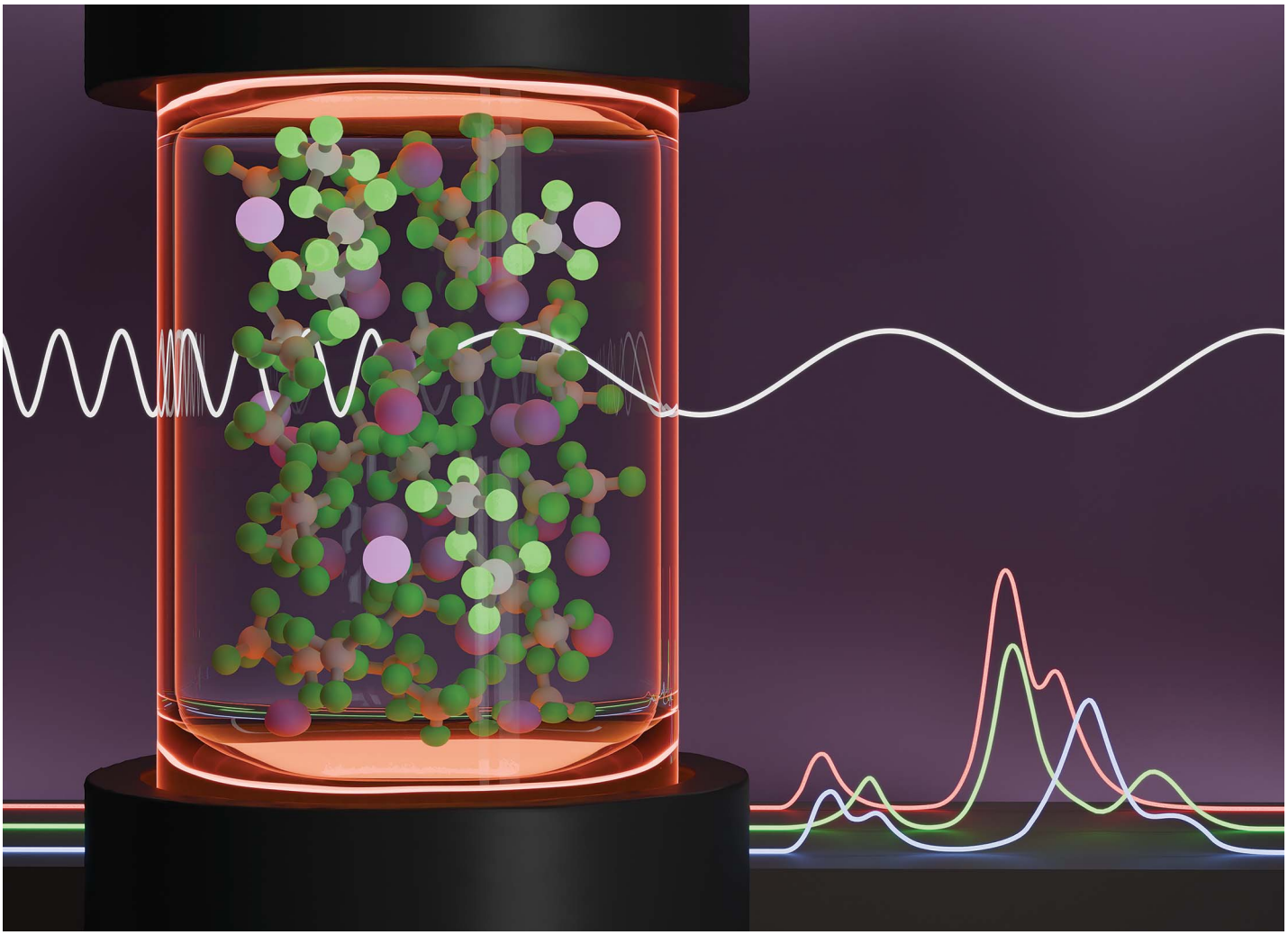
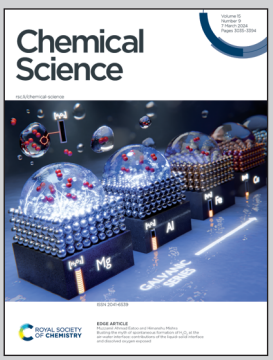


Showcasing research from the groups of Dr. Santanu Roy and Dr. Vyacheslav S. Bryantsev at Oak Ridge National Laboratory, Oak Ridge, USA.

Tracing mechanistic pathways and reaction kinetics toward equilibrium in reactive molten salts

In this work, the complex speciation of a highly reactive molten salt mixture ($AlCl_3$-KCl) is revealed through extensive *ab initio* modelling. For a range of compositions, we identify multiple competing reaction pathways and characterize their kinetics with a Marcus-like rate theory. The dynamic speciation in each composition is analysed using simulated spectroscopy and scattering methods. Notably, we demonstrate how simulated Raman spectroscopy outperforms the computed neutron structure factor, S(q), at recognizing changes in speciation. By benchmarking against experiment, simulated Raman spectra identify the true distributions of species at equilibrium.

As featured in:



See Santanu Roy, Vyacheslav S. Bryantsev *et al.*, *Chem. Sci.*, 2024, **15**, 3116.

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