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MULTISCALE MODELLING OF ELECTROCHEMICALLY ACTIVE MATERIAL SYSTEMS: FROM SERVICE TO RECOVERY IN A CIRCULAR ECONOMY

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ABSTRACT

Charge-transfer and redox reactions, and the solid-state processes they drive, shape the behaviour of materials throughout the life cycle of engineered components. They govern the performance and ageing of batteries, electrolysers and fuel cells; contribute to corrosion, hydrogen uptake and embrittlement; and enable end-of-life material recovery, including the hydrogen decrepitation of rare-earth magnets. By linking longer service life with more effective material recovery, the two principal levers of a circular economy, this session highlights the shared physical principles underlying durability, degradation and recycling.

These processes share a common mathematical and computational structure: transport of charged species, nonlinear interface kinetics, and coupling to mechanics through swelling, stress-assisted diffusion and fracture. Their modelling spans the molecular, microstructural and component scales. The resulting systems are multiscale, stiff, often posed on evolving domains such as dissolution fronts and cracks, and depend on parameters that must be inferred from sparse and noisy data. The session brings together communities that meet these challenges separately, so that methods developed in one field reach the others. It addresses the conference themes of energy systems, clean mobility, and waste and resource management.

Topics include: (i) models of corrosion and corrosion inhibition, from the molecular design of inhibitors to passive films and protective coatings; (ii) hydrogen uptake, transport, trapping and embrittlement; (iii) electro-chemo-mechanical degradation of batteries, electrolysers and fuel cells; (iv) phase-field, cohesive-zone and unfitted methods for fracture and moving interfaces; (v) electrochemical and solid-state processes for recycling and material recovery; (vi) scale bridging, surrogate modelling, Bayesian calibration and uncertainty quantification; and (vii) digital twins for lifetime prediction. Contributions that confront models with experiments, and contributions from industry and public stakeholders, are particularly welcome.