Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally Mandal, Ranga Reddy Dist., Hyderabad – 500 046

Seminar

From Rechargeable Battery Diagnostics to Molecular Dynamics

Alexej Jerschow

New York University, NY

Rechargeable batteries pose significant challenges for nondestructive characterisation due to their complex internal dynamics and failure mechanisms. We present advanced diagnostic approaches that leverage magnetic resonance and magnetometry techniques, complemented by molecular dynamics (MD) simulations, to provide deep insights into battery processes across multiple length and time scales. MRI-based methods enable fast, spatially resolved, nondestructive scanning of full cells, allowing sensitive determination of site-resolved state-of-charge, current distributions, early defect detection, and electrode chemistry changes during charge/discharge cycles. To further elucidate underlying dynamic processes, we integrate NMR spectroscopy, which probes motions over wide timescales (ps to μs) via relaxation rates, with MD simulations. This synergy enables rigorous untangling of relaxation mechanisms, elucidating dynamical models on molecular scales, and enhancing signal assignment. Recent extensions include tracking sodium ions in hydrogel-based desalination materials. Overall, the combined use of MRI, magnetometry, advanced NMR, and MD simulations provide powerful methodologies for fundamental electrochemical research, and accelerated development of next-generation of materials and devices.

Friday, Jan 23rd 2026

16:00 Hrs (Tea / Coffee 15:45 Hrs)

Auditorium, TIFRH