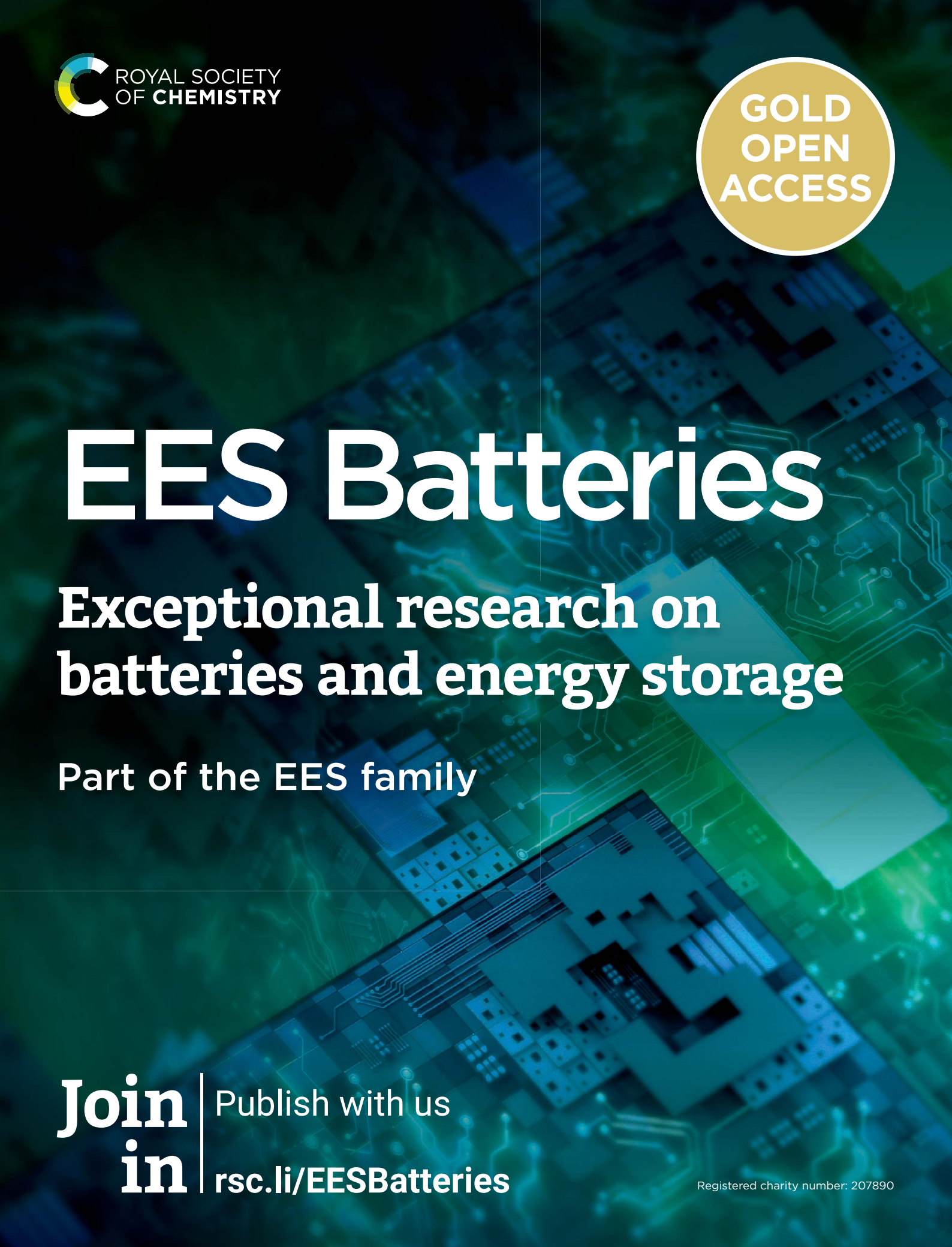
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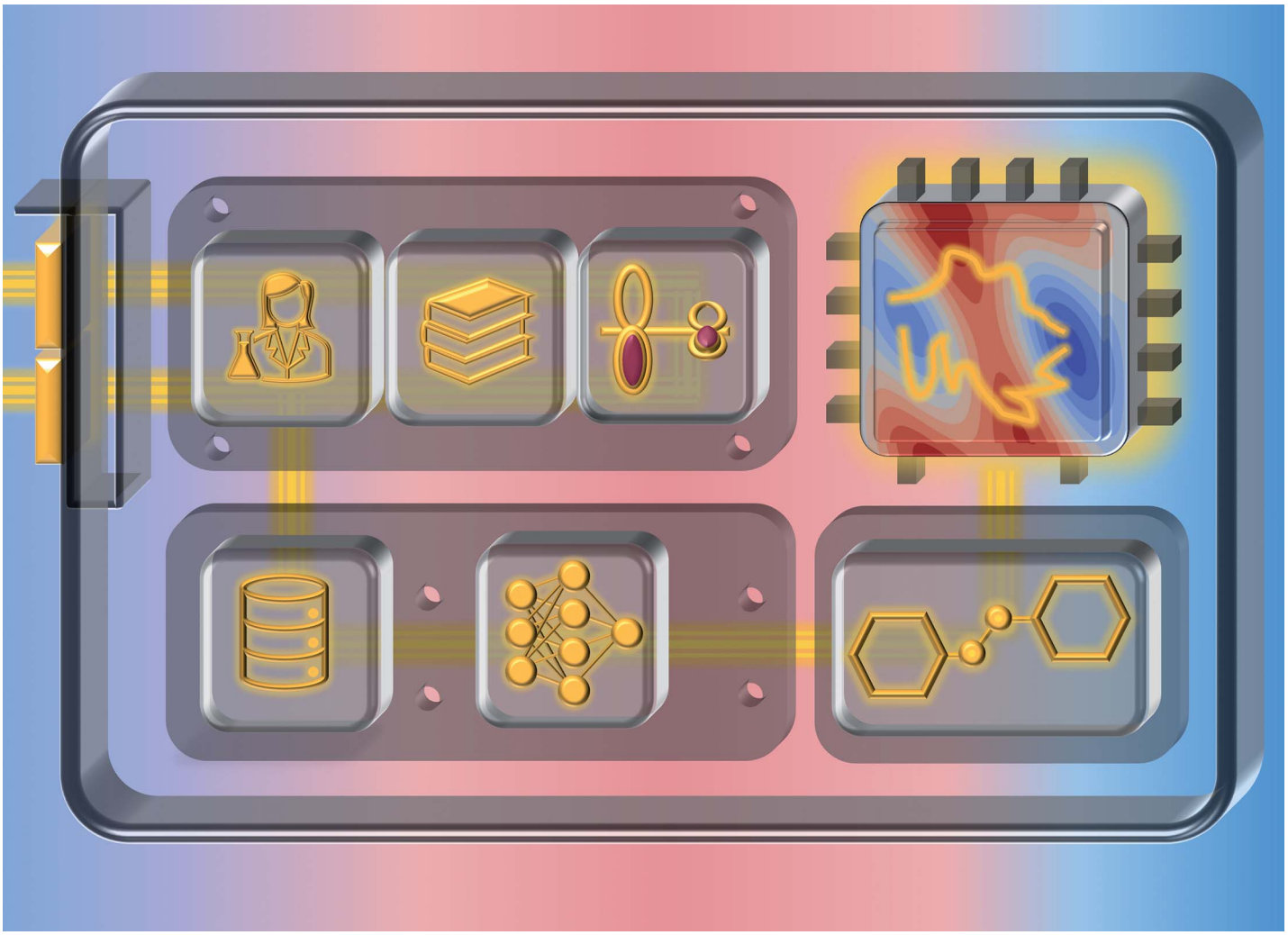

Showcasing research led by Dr. Nikita Fedik and collaborators from Los Alamos National Laboratory, New Mexico, US.

Challenges and opportunities for machine learning potentials in transition path sampling: alanine dipeptide and azobenzene studies

One of the focuses of our team is the development and applications of machine learning interatomic potentials for advancing the simulations of chemical properties. In this study, we show that general-purpose ML potentials can capture interconversion trajectories and potential energy surfaces in systems like alanine dipeptide. However, for more complex molecules such as azobenzene, where bond breaking and electronic effects accompany isomerization, domain expertise and adequate level of reference theory are essential to ensure realistic modelling and get insights into the model accuracy.

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As featured in:

See Nikita Fedik *et al.*, *Digital Discovery*, 2025, **4**, 1158.

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