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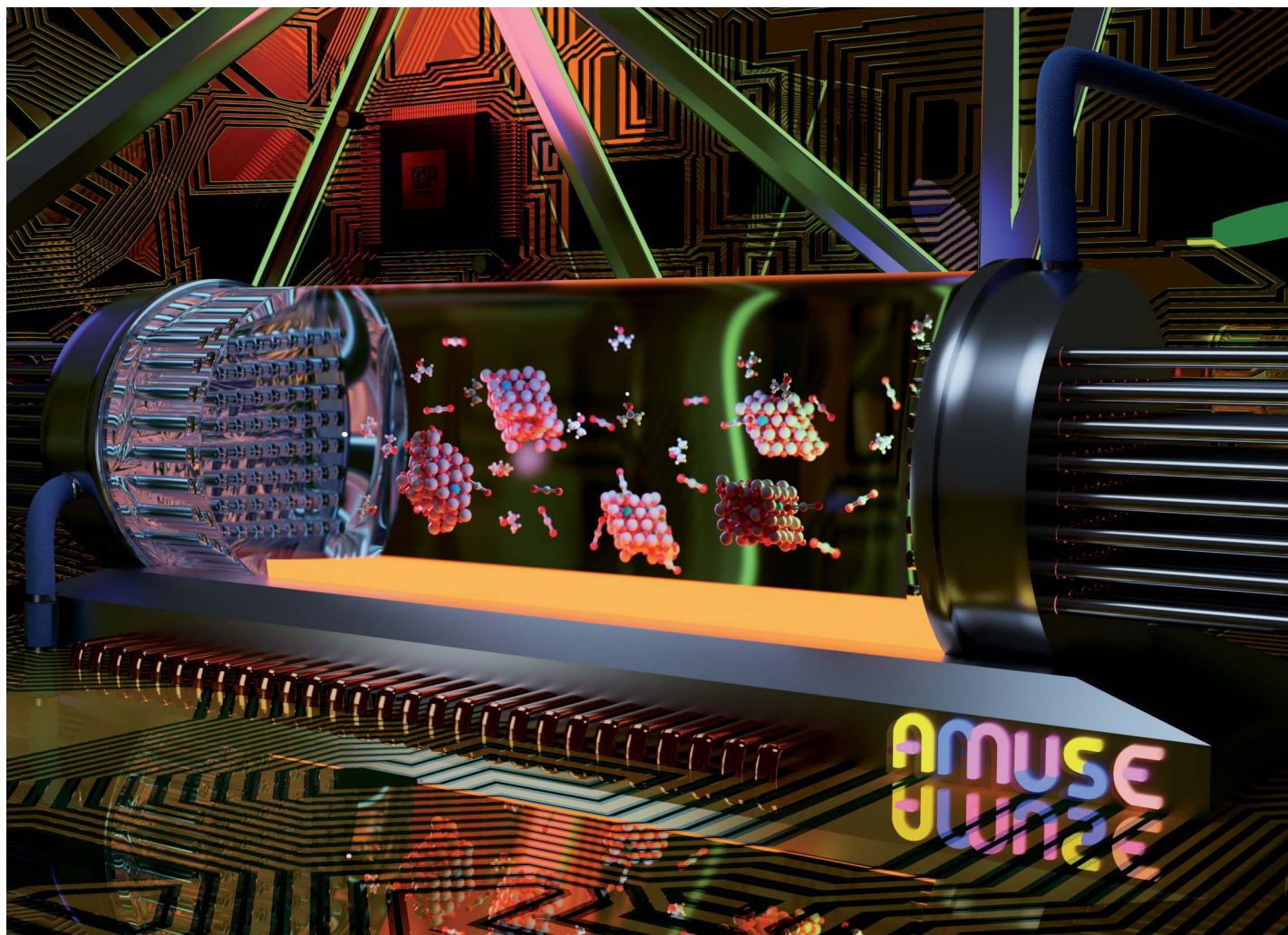
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Showcasing research from Professor Núria López's Computational laboratory, Institute of Chemical Research of Catalonia (ICIQ-CERCA), Tarragona, Spain.

Automated MULTiscale simulation environment

The Automated MULTiscale Simulation Environment or AMUSE is a multiscale framework integrating detailed atomistic information on materials and reactions to predict the performance of heterogeneous catalytic full-scale reactors. The code is modular, and each one of its functionalities can be used separately and can be found in the following GitHub repository: <https://github.com/LopezGroup-ICIQ/amuse/tree/main>. AMUSE has been applied in the study of two industrially relevant reactions: iso-propanol dehydrogenation and CO₂ hydrogenation. The accuracy of the obtained results confirms the potential of this tool.

As featured in:



See Albert Sabadell-Rendón, Núria López *et al.*, *Digital Discovery*, 2023, 2, 1721.