

Can AI See Molecules Dance?

A breakthrough in real-time liquid chemistry reveals new energy pathways.

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658

Nature article number

Published in the October 12, 2026, issue of Nature, this study marks a pivotal moment in observing molecular behavior in solution.

The study, published in Nature 658, demonstrates how time-resolved X-ray liquidography captures ultrafast molecular motions during a classic photoisomerization reaction. This technique allows scientists to observe how azobenzene molecules reconfigure in real time—critical for designing light-responsive materials used in solar energy conversion and molecular electronics. The resolution achieved surpasses previous methods, enabling AI models to simulate complex energy-transfer pathways with unprecedented fidelity.

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https://www.nature.com/articles/d41586-026-02970-y?error=cookies_not_supported&code=8b7a1f50-4b03-49a4-8ef9-611b9ad62ce3



01

AI learns from molecular chaos

Unlike traditional simulations that assume idealized environments, this data reflects the true complexity of liquid-phase reactions—where solvent molecules constantly perturb the system. AI trained on such data can generalize better across diverse chemical environments, a critical capability for modeling energy systems under fluctuating real-world conditions.

02

From lab to grid: AI as molecular architect

This approach mirrors how AI optimizes data-center cooling by modeling airflow in real time. Here, the 'cooling' is molecular stability; the 'load' is energy transfer efficiency. The same AI architecture used to balance server workloads can now be applied to stabilize reactive intermediates in photochemical reactions—turning AI into a true co-designer of next-gen energy materials.



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