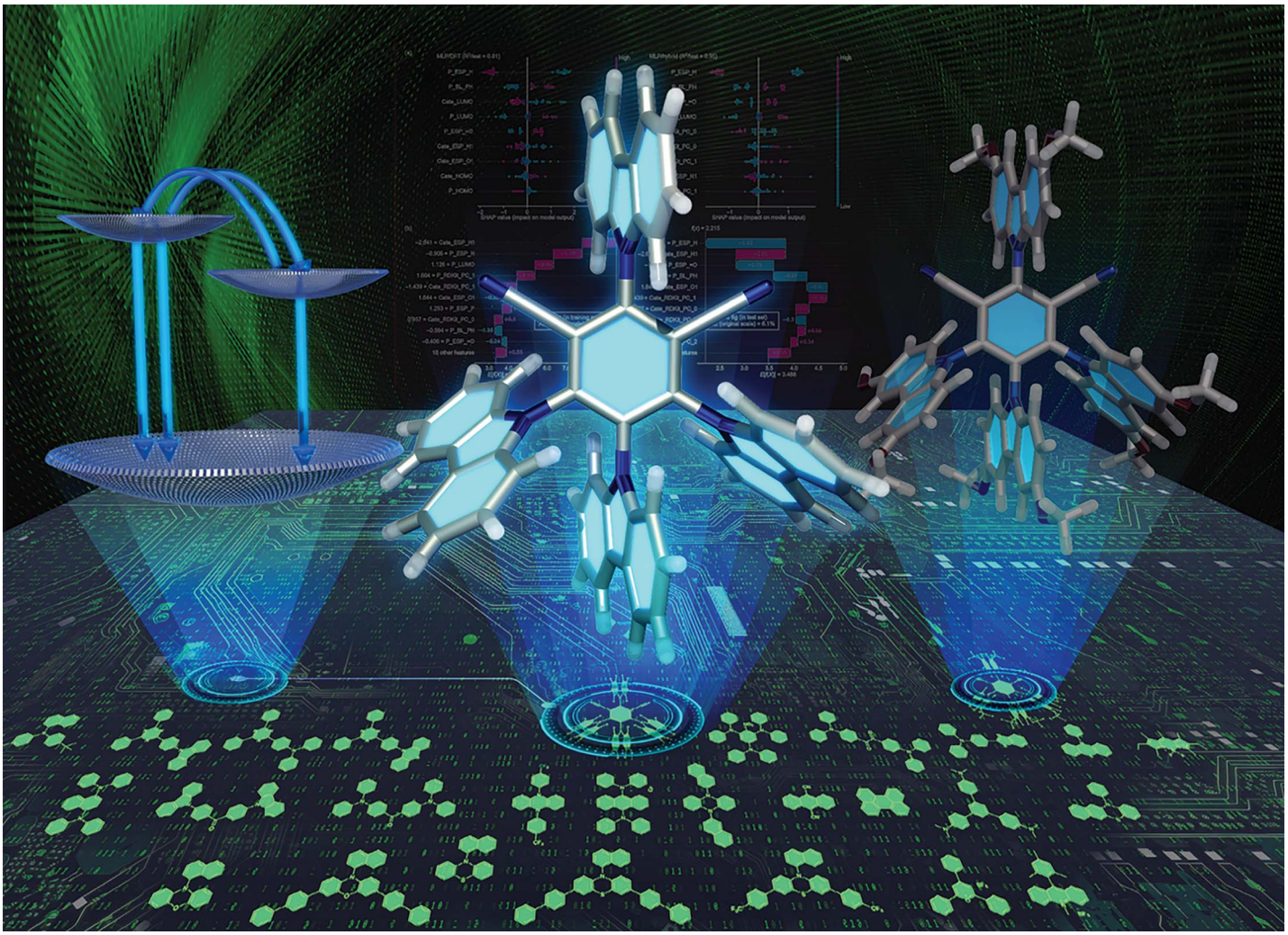

**Showcasing research from Professor Saito's laboratory, Department of Chemistry, Nagoya University, Aichi, Japan.**

Data-driven approach to elucidate the correlation between photocatalytic activity and rate constants from excited states

This work presents a data-driven framework that uncovers how excited-state kinetics govern the catalytic activity of organic photosensitizers by integrating machine learning with quantum chemical calculations. Theoretically simulated rate constants from excited states were shown to outperform experimentally measured excited-state lifetimes as descriptors. SHAP-based visual analyses revealed that transitions from the $T_1$ state, together with the non-radiative decay process between the $S_1$ and $S_0$ states, play key roles in determining photocatalytic activity. This computational approach provides insights that are not readily accessible through conventional experimental methods.

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## As featured in:


See Naoki Noto, Takeshi Yanai, and Susumu Saito *et al.*, *Chem. Sci.*, 2026, **17**, 176.

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