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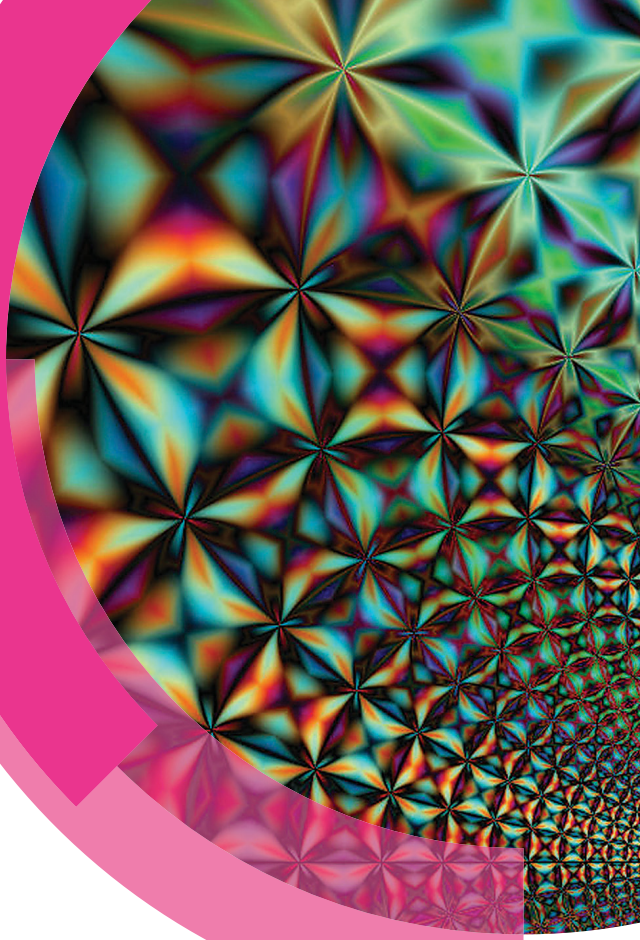

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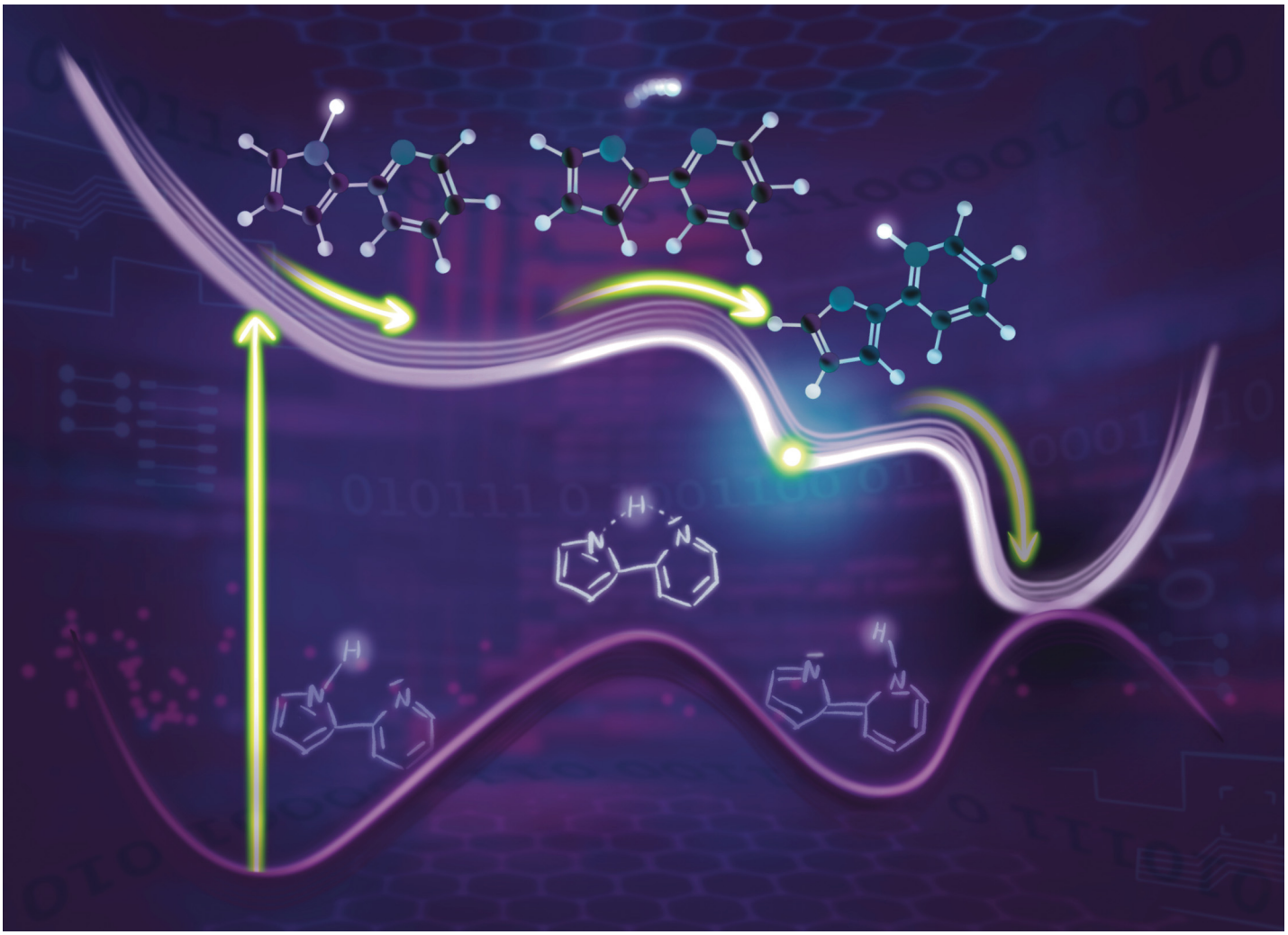

Showcasing research from the Group of Dr Morgane Vacher at CEISAM Laboratory, CNRS - Nantes Université, France.

ESIPT in the pyrrol pyridine molecule: mechanism, timescale and yield revealed using dynamics simulations

This work features extensive investigation of the Excited State Intramolecular Proton Transfer (ESIPT) reaction of the 2-(1*H*-pyrrol-2-yl)pyridine molecule using non-adiabatic dynamics simulations. Two complementary mechanisms are found to drive the proton transfer. First, the initial geometrical relaxation of the excited system leads to a large and fast proton transfer. Then, lingering coherent oscillatory motion in the reactant excited well yields periodic-like increases in proton transfer rate. The significant fluorescence quenching of the photo-product *via* non-radiative relaxation is also assessed.

As featured in:

See Morgane Vacher *et al.*, *Phys. Chem. Chem. Phys.*, 2023, **25**, 9761.

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