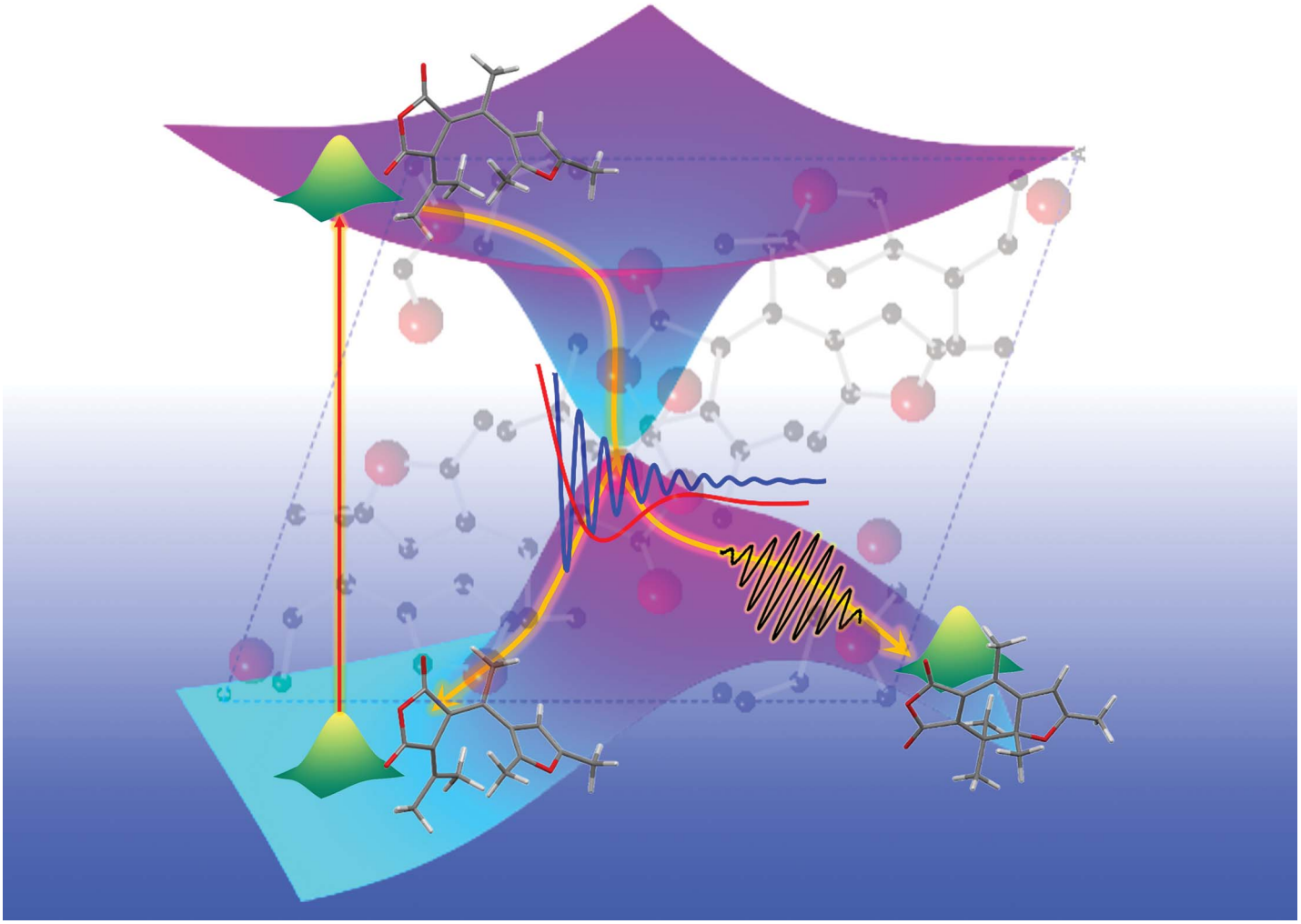

Showcasing research from Professor R. J. Dwayne Miller's laboratory, Departments of Chemistry and Physics, University of Toronto, Toronto, Canada.

Elucidating the reaction kernel and probing the effect of anharmonicity in the ring-closing reaction of fulgide single crystals

Chemistry involves dynamics that bridge structural changes. Among the vast milieu of quantum vibrations, it ultimately comes down to a few key motions that drive the system across the transition state, defining the reaction kernel. It is the anharmonicity at the barrier-crossing region that couples normal modes, leading to localized motions and reduced dimensionality. In this study, we have elucidated the reaction kernel for the ring-closing reaction in fulgide single-crystals. This work unveiled a non-impulsive, coherent vibrational energy transfer mechanism that further highlights the highly anharmonic nature of the potential in reactive crossings that is responsible for the collapse of the system onto a few highly nonlinearly coupled coordinates.

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See Zheng Li, R. J. Dwayne Miller *et al.*, *Chem. Sci.*, 2025, **16**, 19118.

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