

RSC Applied Interfaces

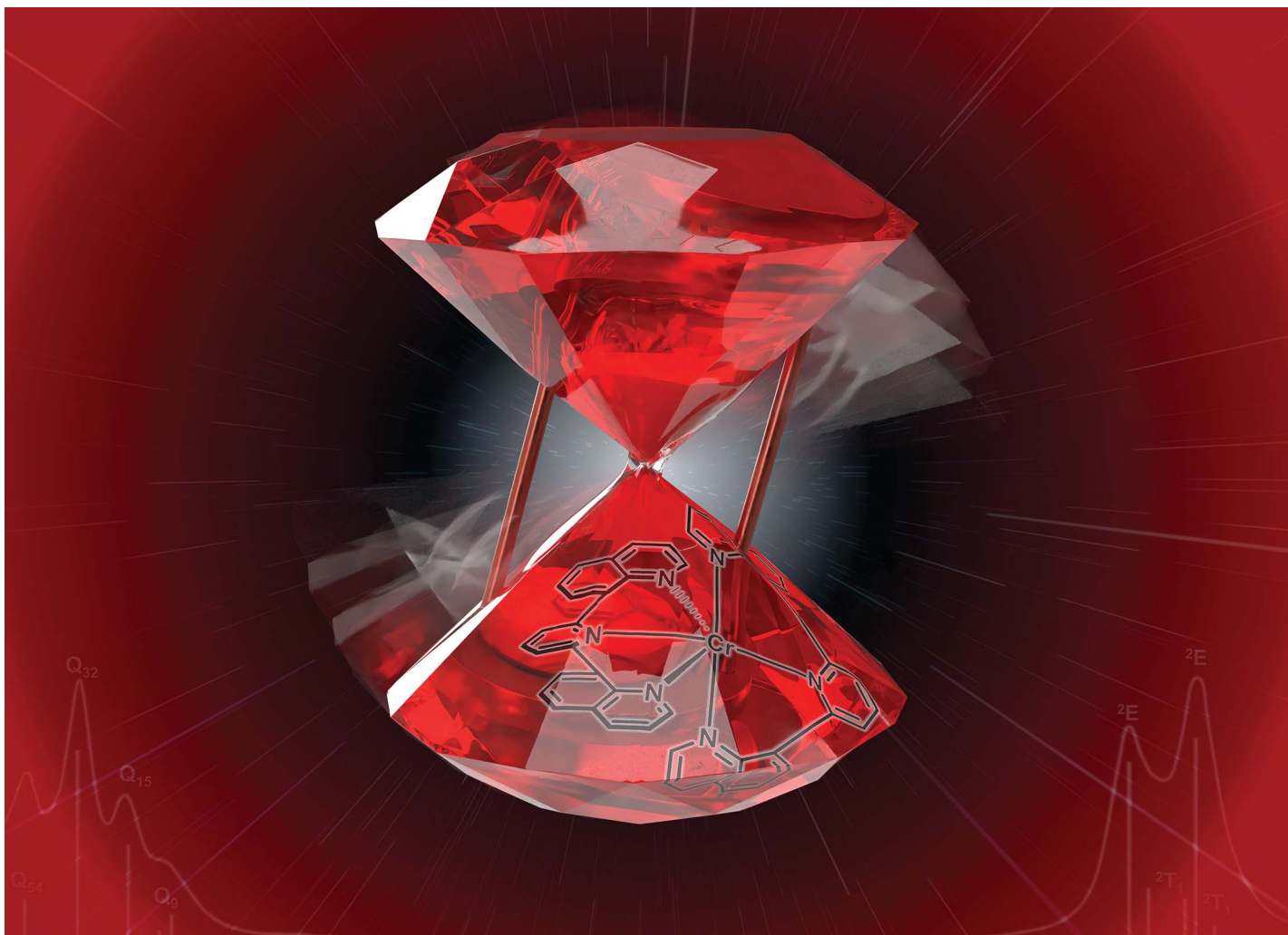
GOLD
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**Interfacial and surface research
with an applied focus**

Interdisciplinary and open access

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**Fundamental questions
Elemental answers**



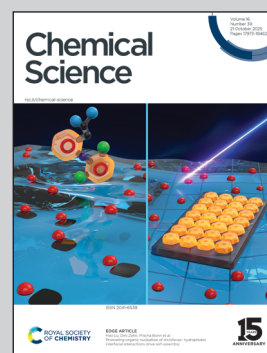
Showcasing research from Dr. Stephan Kupfer's laboratory,
Institute of Physical Chemistry, Friedrich-Schiller-University
Jena, Germany.

Unraveling the photoredox chemistry of a molecular ruby

In-depth computational modelling using state-of-the-art multiconfigurational methods allowed us to elucidate the photophysical processes as well as their kinetics in a Cr(III) spin-flip complex. Particular emphasis was set on investigating various intersystem crossing channels connecting the respective quartet and doublet spin states. Furthermore, ab initio molecular dynamics allowed us to evaluate the photoredox chemistry of the millisecond lived excited molecular ruby in combination with a reductive quencher.

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As featured in:



See Georgina E. Shillito,
Stephan Kupfer *et al.*,
Chem. Sci., 2025, **16**, 18113.