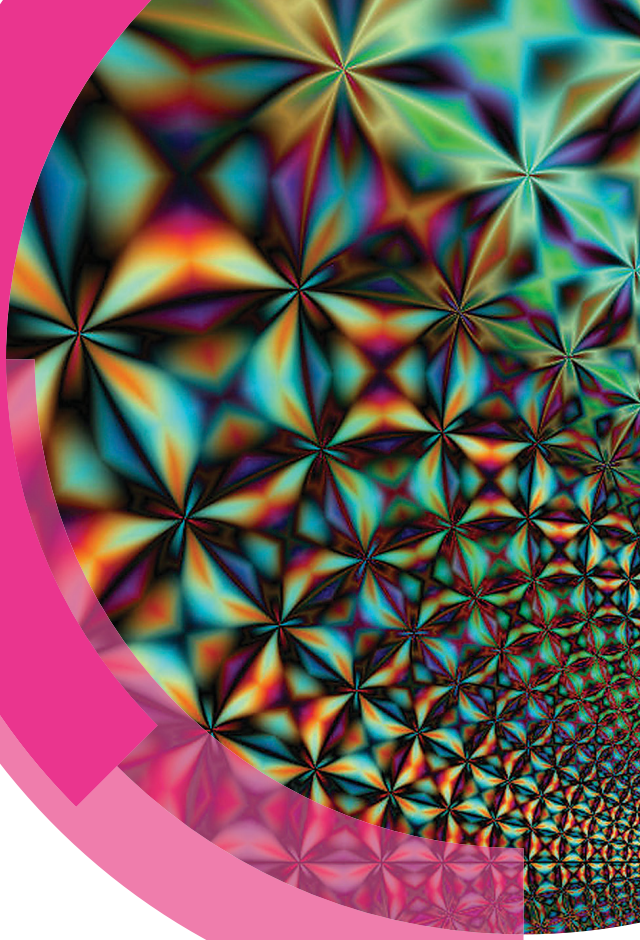
ROYAL SOCIETY OF CHEMISTRY



RSC Advances

At the heart of open access for the global chemistry community

Editor-in-chief

Russell J Cox
Leibniz Universität Hannover, Germany

We stand for:

Breadth We publish work in all areas of chemistry and reach a global readership

Affordability Low APCs, discounts and waivers make publishing open access achievable and sustainable

Quality Research to advance the chemical sciences undergoes rigorous peer review for a trusted, society-run journal

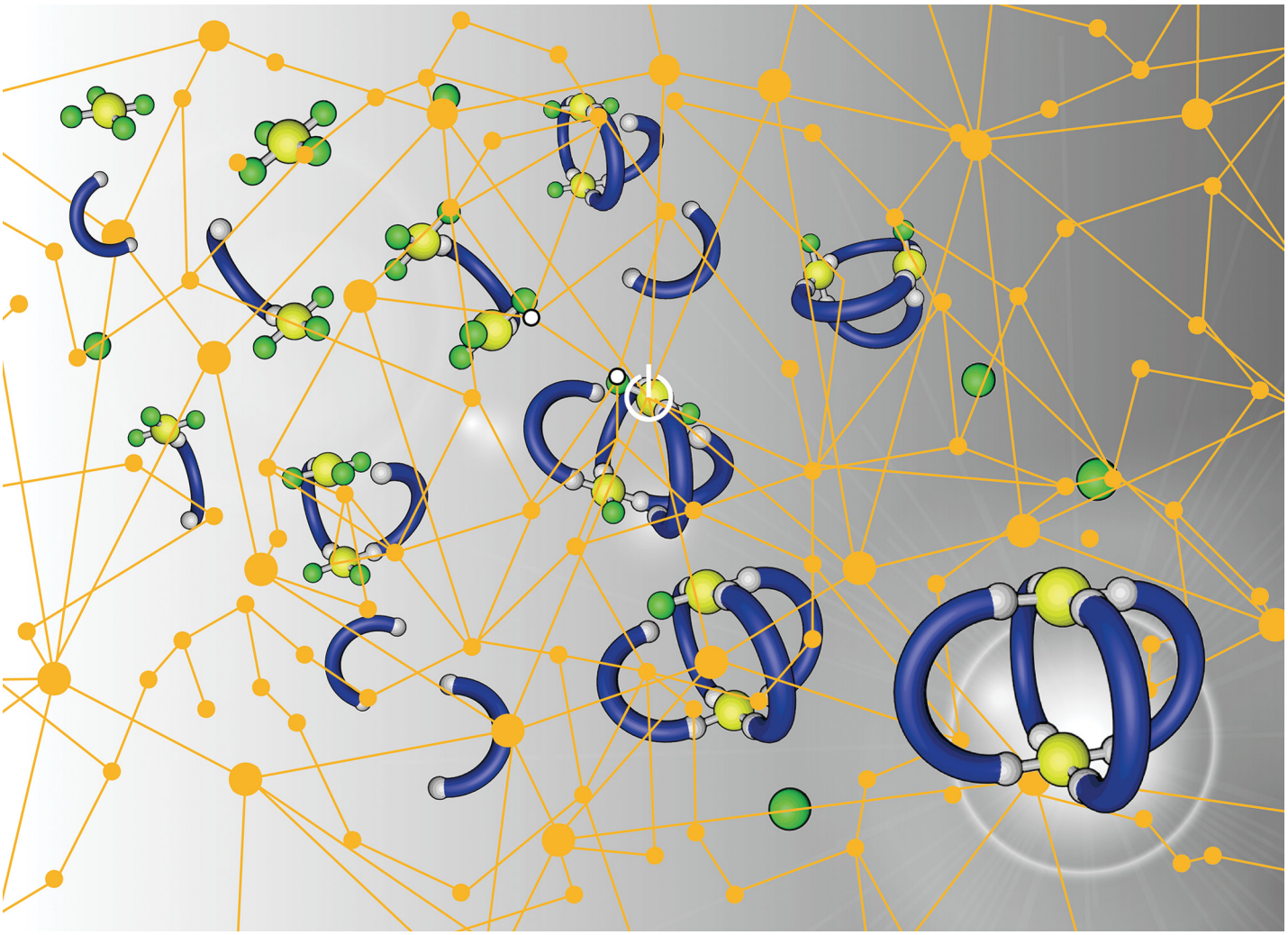
Community Led by active researchers, we publish quality work from scientists at every career stage, and all countries

Submit your work now

rsc.li/rsc-advances

@RSC_Adv

Registered charity number: 207890



Showcasing the perspective from the groups of Prof. Shuichi Hiraoka at the University of Tokyo, Dr Satoru Iuchi at Nagoya University, and Prof. Hirofumi Sato at Kyoto University, Japan.

Theoretical and computational methodologies for understanding coordination self-assembly complexes

Three methods to capture the coordination self-assembly processes at the molecular level are highlighted: quantum chemical modeling, molecular dynamics, and reaction network analysis, covering different scales from the metal–ligand bond to a more global reaction network theoretically and computationally. Suitable numerical approaches to analyze the coordination self-assembly from different perspectives are introduced. Studies based on these methods are paving the way to elucidate increasingly more aspects of the coordination self-assembly.

As featured in:

See Satoshi Takahashi, Hirofumi Sato *et al.*, *Phys. Chem. Chem. Phys.*, 2023, **25**, 14659.

ROYAL SOCIETY OF CHEMISTRY

rsc.li/pccp

Registered charity number: 207890