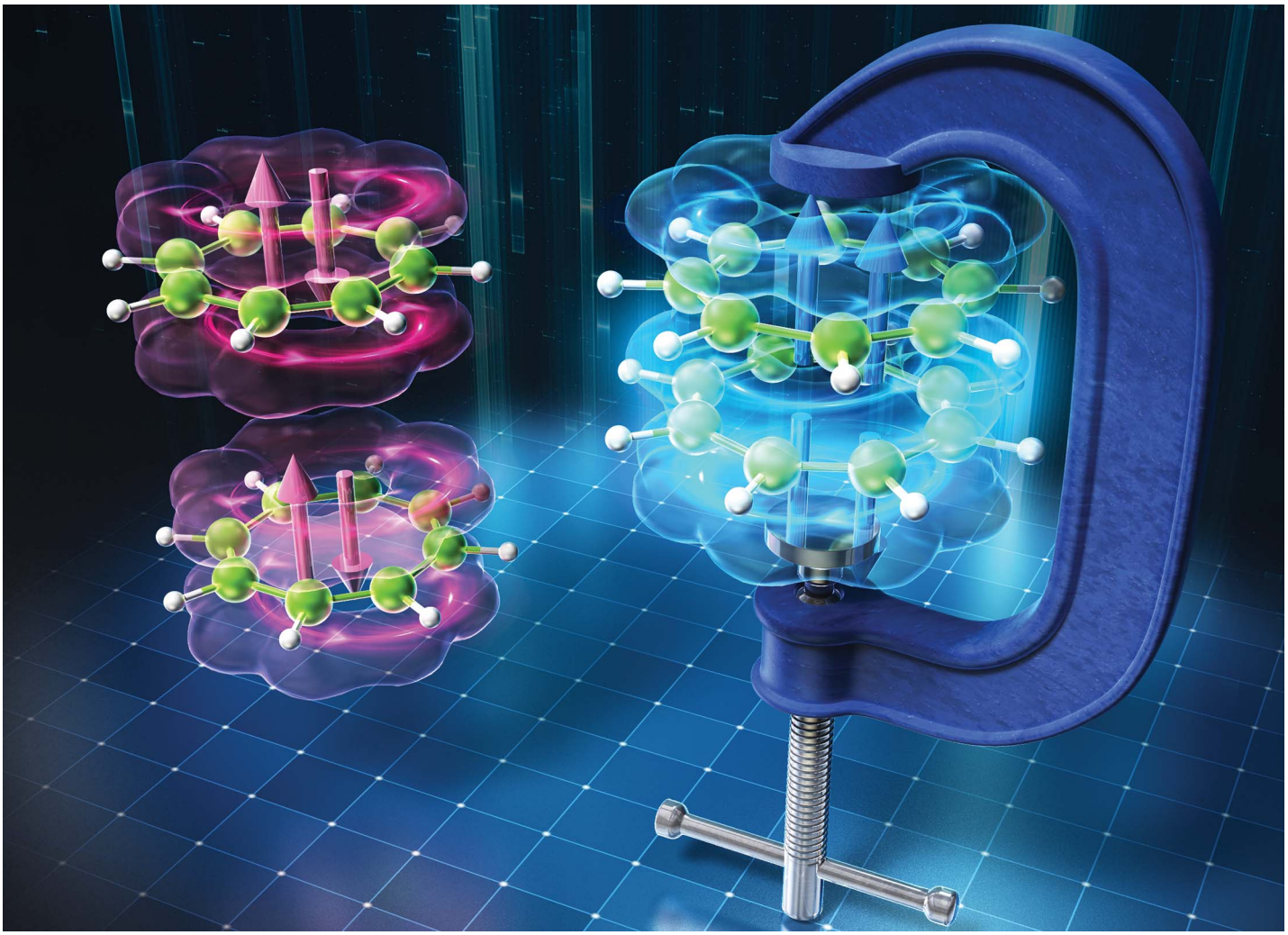

**Showcasing research from Professor Kitagawa's laboratory, Graduate School of Engineering Science, Osaka University, Osaka, Japan.**

Stacked-ring aromaticity from the viewpoint of the effective number of π-electrons

High-level quantum chemical calculations combined with a multi-configurational wavefunction analysis for closely stacked π-dimers of antiaromatic molecules have revealed that the appearance of the double-triplet [$^1(T_1T_1)$] character is critical to connecting the stacked-ring aromaticity concept with Baird's rule. Unpaired electrons derived from the $T_1$-like Baird-aromatic monomers contribute to the formation of intermolecular double bonds through the increased contribution of intermolecular charge-transfer (CT) configurations in the ground state of the π-dimers.

## As featured in:


See Ryota Sugimori, Kenji Okada, Ryohei Kishi and Yasutaka Kitagawa, *Chem. Sci.,* 2025, **16**, 1707.

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