

Haruta has been developing chemical theories for dynamical symmetry, mechanochemistry, and exciton relaxation on the basis of a comprehensive understanding of structures, deformations, and electronic states.

(1) Polyatomic clusters with as-yet-unknown symmetry

He has identified polyatomic clusters with catalytic activity [[Nature Commun. 8, 688 \(2017\)](#)], chemical stability [[Nature Commun. 8, 2046 \(2017\)](#)], and spectroscopic feature [[Science Adv. 5, eaax6455 \(2019\)](#)] in collaboration with experimentalists. Such clusters have been predicted on the assumption that they are spherical, but it is effective just for subglobular clusters such as icosahedron. He proposed a symmetry-adapted orbital model, which incorporates orbital splittings due to lower structural symmetries [[Nature Commun. 10, 3727 \(2019\)](#)]. This refinement predicts an abundance of clusters with various shapes, which obey a certain periodicity. In fact, experimentally observed clusters are governed by the same rule. Consequently, he constructed a periodic framework for clusters, which will be a useful compass to find missing species.

Besides, he theoretically found special clusters. Spherical atoms have the highest geometrical symmetry, and hence atomic orbitals are highly degenerate. As for polyatomic species, an icosahedral structure is the most symmetrical, yielding 5-fold degeneracy at the maximum. He discovered that it is possible to overcome these limitations. Tetrahedral clusters of Mg, Zn, and Cd exhibit higher-fold orbital degeneracy than spherical or icosahedral symmetry [[Nature Commun. 9, 3758 \(2018\)](#)]. Remarkably, the origin of the “super-degeneracy” was identified as “dynamical symmetry”, the superordinate concept of point group. This achievement will lead to supreme conductivity or magnetism utilizing super-degenerate orbitals.

(2) Mechanochemical reactions

He has tackled with mechanically-driven solid-state reactions [[Tetrahedron Lett. 54, 5920 \(2013\)](#); [ChemistrySelect 1, 984 \(2016\)](#); [Tetrahedron 73, 2305 \(2017\)](#)], and successfully elucidated how mechanical action opens a new reaction path. Dibenzophenazine was recently synthesized in a ball-milling way at a high yield. This synthesis was expected to involve two distinct reaction paths. Actually, DFT calculations show a stepwise lowest-energy path and also a concerted one with a higher barrier. However, the highest energy point along the latter path is not a transition state but a higher-order saddle point. The concerted path is therefore not generally accepted as a reaction path. He found that mechanical force causes molecular deformation and removes the instability so that the higher-order saddle point is changed into a transition state [[J. Phys. Chem. C 123, 21581 \(2019\)](#)].

(3) A novel type of long-lived excitons

He has also solved a problem related to exciton dynamics in organic LEDs. A bisanthracene derivative is known as an excellent luminescent material. Its high efficiency, however, cannot be explained by conventional thermally activated delayed fluorescence nor triplet-triplet annihilation. He focused on its pseudo-degenerate frontier orbitals. His unexpected finding is that pseudo-degeneracy generally suppresses nonradiative transitions, owing to the nontrivial cancellation of overlap between many-electron wave functions [[Sci. Rep. 7, 4820 \(2017\)](#); [J. Mater. Chem. C 7, 2541 \(2019\)](#)]. As for the bisanthracene derivative, electrically generated “higher triplets” are thus long-lived, and then converted into a fluorescent singlet. His discovery tells us a novel category of efficient organic LEDs.