Inverse Design Approach for Molecular Aggregates and Molecule-Nanoparticle Systems

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Photophysical properties of molecules can be enhanced in the molecular aggregates and near the nanoparticles (NPs). Here, we propose the theoretical design approach for the photofunctions of molecular aggregates [1] and molecule-NP systems [2] using the inverse design framework.

For molecular aggregates, Frenkel exciton model coupled with a linear combination of atomic potentials is introduced for designing systems with desired optical properties by gradient-guided optimization searches in terms of constituent molecules in chemical space of molecular aggregates. We have applied this approach to design one-dimensional molecular aggregates having maximized absorption and/or circular dichroism intensities. By exploring a small fraction of the vast chemical space of 10^{26} possible systems varying in composition and structure, we successfully obtained the optimal aggregates.

We also proposed an inverse design method of the optimal molecule–NP systems and incident electric field for the desired photophysical properties by the gradient-based optimization search within the time-dependent quantum chemical description for the molecule and the continuum model for the metal NP. We designed the optimal molecule, molecule–NP spatial conformation, and incident electric field to maximize the population transfer to the target electronic state of the molecule.

We will also introduce our recent work on coordination asymmetry of C@Au6 clusters.

[1] T. Shiraogawa, M. Ehara, *J. Phys. Chem. C* **124**, 13329 (2020).

[2] T. Shiraogawa, M. Ehara, G. Dall'Osto, R. Cammi, M. Ehara, S. Corni, *Phys. Chem. Chem. Phys.* **24**, 22768 (2022).