第441回触媒科学研究所コロキウム

Classical and Quantum Mechanical Simulations of Optical Properties of Metal Clusters

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Optical properties of ligand-protected metal clusters are employed in a great many applications that include notably as electrocatalysts for energy conversion, and also biomedical uses. The interaction between the ligands and the metallic cores, mediated by an often complex interface, profoundly influences the properties of small clusters, in particular. Nonetheless, the mechanisms of interaction remain far from fully understood. To this end, in this presentation I talk about simulations by means of Fourier-transformed induced densities from real-time (time evolution) calculations of time-dependent density-functional theory (TDDFT). Two different test-case systems will be presented: the $Au_{144}L_{60}$ class of cluster compounds for which total structure determination has been achieved only recently for a thiolated and an all-alkynyl cluster, and the $Ag_{29}(BDT)_{12}(TPP)_4$ cluster, the geometry of which is also available from experimental structure determination.

He obtained PhD in condensed matter physics in 2018 from Aix-Marseille University, France and Autonomous University of Madrid, Spain. 2018-2019: Postdoctoral Resercher. CEMES, CNRS, Toulouse, France. 2019-2020: Postdoctoral Resercher. CNRS, CINaM, Marseille, France. Since June 2020: Postdoctoral Resercher. École Polytechnique, LSI, Palaiseau, France. In 2021, he obtained the scholarship from the Japan Society for the Promotion of Science (JSPS) to start collaboration with Prof. Kazuhiro Yabana at Tsukuba University. Recently, he obtained the position of Asst. Prof. in Univ. Valuse Bernard Lyon1, Lyon, France.

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