

## **Unraveling the charge transfer mystery in mix-valence compounds**

Charge transfer is a fundamental reaction in which a charge moves from a donor, where there is an excess of charge, to an acceptor, where there is a charge deficiency. This process plays a crucial role in various biological reactions that determine the functioning of living organisms on our planet, such as photosynthesis. Additionally, charge transfer finds applications in modern technologies, such as photovoltaics.

Chemical systems where charge transfer occurs are called mixed-valence compounds, encompassing organic and inorganic molecules, metal complexes, and solids. Investigating mixed-valence compounds is essential for better understanding, optimizing, and controlling the charge transfer process. Quantum chemistry methods serve as powerful tools for studying charge transfer at the molecular level. These methods provide detailed information about molecular geometry and precise descriptions of electronic structures. Such information can be utilized to determine the charge's location within the chemical system and characterize its nature, whether it is localized on the donor or acceptor or delocalized between them.

The research will employ various quantum chemical methods to accurately describe the location and degree of charge localization in small diamine cations. The migration of a charge influences changes in the system's geometric and electronic structures. Throughout the project, the initial, transition, and final states along the reaction path of the investigated diamine cations will be examined regarding their geometries, electronic structures, and energies. These studies will contribute to determining the mechanism of the charge transfer process in diamine cations.

Successful completion of this project will enhance our understanding of the potential mechanisms underlying charge transfer processes between donors and acceptors from a molecular perspective. A charge transfer is a fundamental reaction that drives vital biological processes. The results of quantum chemistry methods can help address uncertainties surrounding complex natural reactions. Moreover, knowledge about charge migration can assist in optimizing and better controlling existing technological devices that rely on the charge transfer process. Investigating mixed-valence compounds, such as diamine cations containing two states with differing levels of charge localization, offers an opportunity to study the performance of quantum chemistry methods in addressing complex electronic structure problems. Additionally, the findings can complement experimental observations of processes occurring within femtoseconds ( $10^{-15}$  s).