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| **Title** | **Quantum information transfer via charge transfer processes** |
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**Project description:**

Quantum Information is a flourisching research area relevant to quantum technologies and quantum phenomena in physics and chemistry. Quantum information science offers opportunities for understanding chemical processes and, vice versa, advanced chemistry can provide ways to handle quantum information through molecular systems and processes [1].

Fundamental questions concern the role of correlations of quantum type (which are fundamental to quantum information) in chemical reactions. For example, is it possible to influence a chemical reaction by creating suitable quantum correlations between the reactants? A recent study has proposed a way to introduce quantum coherence between the donor and acceptor states of a charge-transfer system, with the goal of gaining control over the charge transfer process and exploiting it to implement quantum gates useful for quamtum computing [2]. Another study has further clarified the picture of a two-state charge-transfer system as a qubit of use in quantum computation and information transfer [3].

This PhD project aims to (a) achieve a deeper understanding and characterization of electron transfer in terms of its quantum information properties; (b) elaborate on the limitations posed to quantum information transfer by the occurrence of decoherence due to the nuclear environment and its interaction with the transferring electron; (c) devise ways to at least partially overcome such limitations and utilize the charge transfer as a means for information transfer and quantum computing.

Techniques from quantum mechanics and quantum chemistry will be combined to develop the theoretical framework and derive the model parameters for selected molecular systems that will be proposed for practical applications.

**References:**

[1] Scholes, G. D. et al., The Quantum Information Science Challenge for Chemistry. J. Phys. Chem. Lett. 2025, 16, 1376.

[2] Migliore, A.; Messina, A. Controlling the charge-transfer dynamics of two-level systems around avoided crossings. J. Chem. Phys. 2024, 160, 084112.

[3] Migliore, A. et al., General Inverse Problem Solution for Two-Level Systems and Its Application to Charge Transfer. Physics 2024, 6, 1171.

**Collaborations/Network:**

Prof. A. Messina (University of Palermo); Prof. H. Nakazato (Waseda University, Japan); Prof. S. Corni (University of Padova); Prof. A. S. M. de Castro (University of Ponta Grossa, Brazil); Prof. A. Sergi (University of Messina).