Quantum Mechanical Model for Long-Range Electron Transport in Solid-State Protein Junctions

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Solid-state electronic junctions of biological macromolecules – from DNA to functionally more diverse proteins – have become of increasing interest given several truly astonishing properties, such as efficient transport of electrons over longer than expected distances[1]. That transport often shows no significant or minimal change when the junctions are cooled to 10 Kelvin or even lower[2].

The potential to incorporate proteins as active elements in electronic devices has thus prompted numerous experimental and theoretical studies to understand the current flow through proteins in solid-state junctions and how to control it. With the rising interest came the awareness that the theoretical description of the electron transport mechanism through these junctions is very challenging because different conductance regimes have been observed depending on the experimental conditions. This situation led to an ongoing debate, highlighting the lack of well-tested theoretical models capable of describing all the different behaviors these systems show.

According to our model[3], for junctions based on ultra-thin films of two types of electron transfer proteins, the conductance at sufficiently low temperatures is no longer dominated by electrons activated from the HOMO to LUMO orbitals. Instead, electrons from the electrode can tunnel into spatially close, localized states of the protein and then, within the protein, descend – in energy – to low-lying states, such as the LUMO and LUMO+1. Electrons escaping from LUMO+1 modulate the conductance with a temperature-dependent contribution with an Arrhenius-like factor.

We could extract the corresponding activation energies and, using advanced DFT calculations[4,5], get the relevant energy differences that match the activation energies well, implying the mechanism's validity.

While our Landauer-based model reproduces the experimental temperature-current results, it is more important and convincing that it explains, for the first time, the empirical observation of how just one of the contacts defines the behavior of the complete junction.

References

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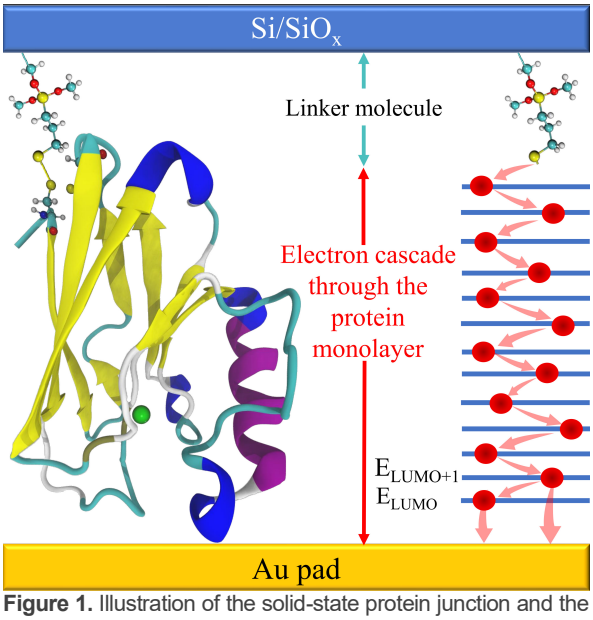

Figure 1. Illustration of the solid-state protein junction and the proposed mechanism.