Coherent electron transport across a 3nm bioelectronic junction made of multi-heme proteins

Zdenek Futera, Ichiro Ide, Ben Kayser, Kavita Garg, Xiuyun Jiang, Jessica H. van Wonderen, Julea N. Butt, Hisao Ishii, Israel Pecht, Mordechai Sheves, David Cahen, and Jochen Blumberger[a]

Affiliation: [a]Department of Physics and Astronomy, University College London, London WC1E 6BT, U.K.

Email: j.blumberger@ucl.ac.uk

Abstract: Multi-heme cytochromes (MHCs) are fascinating proteins used by bacterial organisms to shuttle electrons within, between, and out of their cells. When placed in solid-state electronic junctions, MHCs support temperature-independent currents over several nanometers that are 3 orders of magnitude higher compared to other redox proteins of similar size. I my talk I will describe how we combined experimental measurements (I-V and photo-emission spectroscopy) with explicit electronic structure calculations (DFT+Σ) on gold-MHC-gold junctions to obtain molecular-level insight into their astonishingly high conductivities. We find that conduction across the dry, 3 nm long protein occurs via off-resonant coherent tunneling, mediated by a large number of protein valence-band orbitals that are strongly delocalized over heme and protein residues. This picture is profoundly different from the electron hopping mechanism induced electrochemically or photochemically under aqueous conditions. Our results imply that the current output in solid-state junctions can be even further increased in resonance, for example, by applying a gate voltage, thus allowing a quantum jump for next-generation bionanoelectronic devices.

References:

[1] Z. Futera et al., *J. Phy. Chem. Lett*, **2020**, *11*, 9766-9774.

Biography: JB is a Professor of Chemical Physics at University College London (UCL) since 2015 and Co-Director of the Thomas Young Centre (TYC), the London Centre for the Theory and Simulation of Materials. Prior to his current appointment he has been a Royal Society University Research Fellow at University of Cambridge, a Lecturer and then Reader in Physics at UCL. His research is focused on the development and application of scale-bridging techniques for the simulation of processes relevant to energy conversion in material science and biology.

Photo