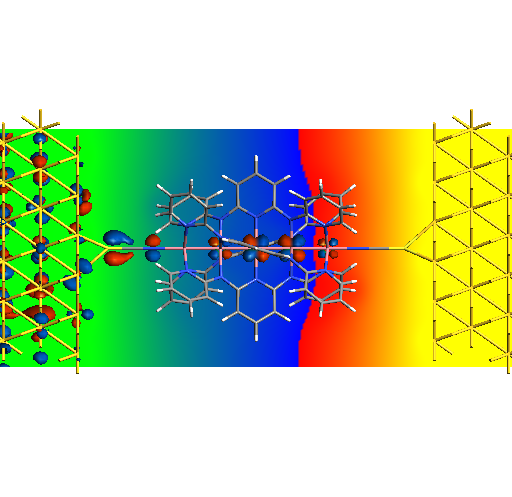
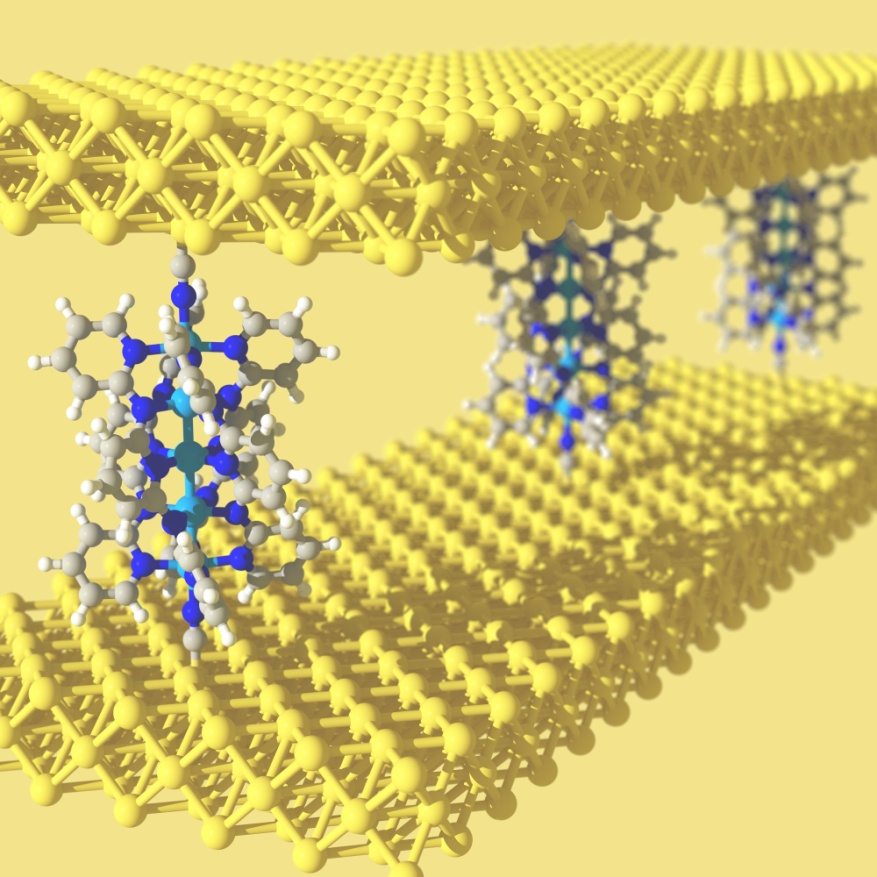
**A theoretical study of electron transport in metal nanowires.**

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Chains of covalently bonded metal atoms offer a striking resemblance to their macroscopic counterparts, but just how real is this resemblance at a quantum level? In this project we aim to use state of the art theory (Density functional theory combined with non-equilibrium Green’s functions) to explore the relationship between structure and function in metal nanowires. The systems of particular interest are the so-called Extended Metal Atom Chains (EMACs), see figure below, where the metal centres range from strongly covalently bonded (Cr3, Ru3, for example) to weakly exchanged coupled (Cu3, Ni3). We will compute from first principles the zero-bias transmission and also the response of the system to applied voltages: past experience suggests that the ground-state electronic structure of these systems is dramatically bias dependent. The project would suit a student with a keen interest in quantum mechanics along with inorganic chemistry and/or materials science.





**References**

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