UNIVERSITY COLLEGE DUBLIN

MNMT-DUBLIN

Periodic Energy Decomposition Analysis For ACSM

Background

Periodic energy decomposition analysis (pEDA) is a theoretical study to understand the interactions happening between two fragments, by evaluating the attractive and repulsive forces, such as electrostatic energy, Pauli's repulsion, orbital and steric interactions. These information help to develop molecular devices by providing a platform to select appropriate molecules as the channel for electronic transport in them.

Industrial demands

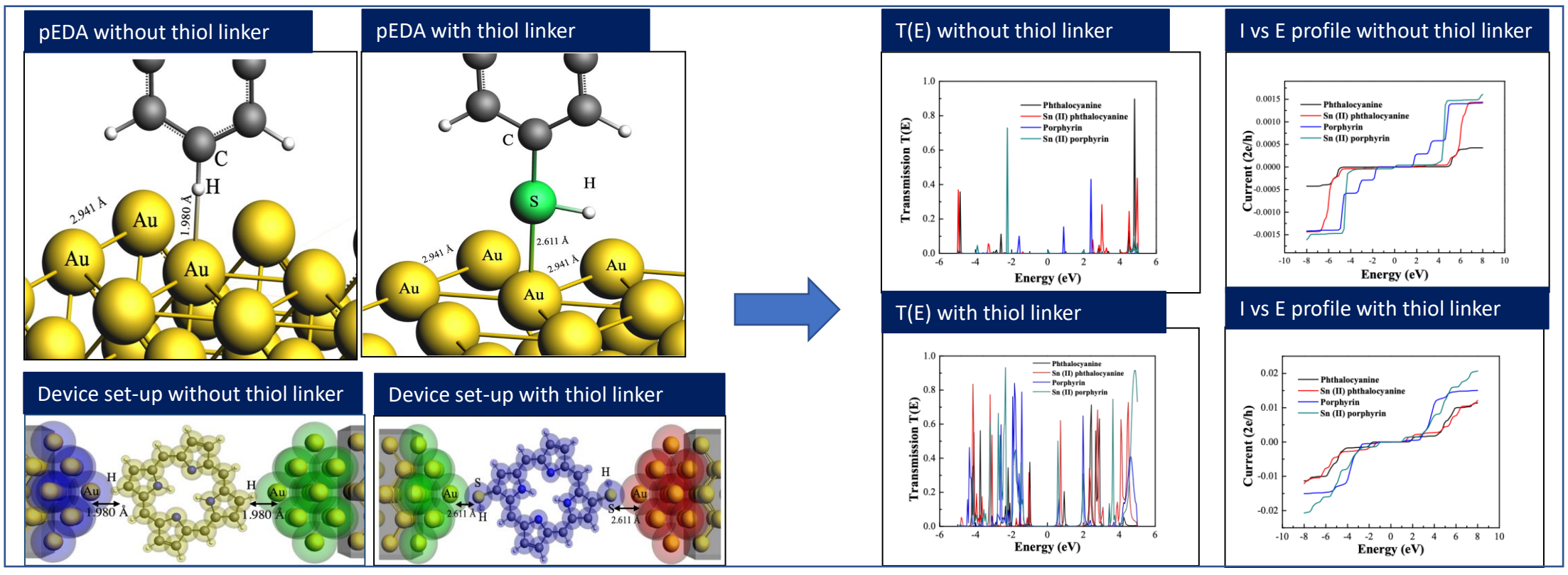
At present, there are over 19 billion transistors in a modern-day chip. The immediate challenge is to develop molecule-based devices to accommodate further electronic components in a chip. For this, suitable molecules should be selected and atomic/close-to-atomic scale electrodes with atomic precision should be fabricated.

New method

MNMT-Dublin has proposed a correlation between pEDA and electronic transport studies, which could aid the selection of molecules and substrates for a stable and robust fabrication of molecular devices in the future.

Progress and results

For the pEDA study, phthalocyanine and porphyrin molecules were selected to understand their behaviour with gold electrodes [Au(111)]. The results show that porphyrins interact with Au better than phthalocyanines. As a result, porphyrins show better transmission [T(E)], when placed between Au electrodes. In addition, both molecules showed a comparable interaction when a terminal thiol linker is attached, which is confirmed by the electronic transmission across the molecular junction. Thus a relation between pEDA and electronic transport study was established.



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