Protocol for unbiased insight into electron transfer in bio-inspired wires

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To better design conductive and bio-compatible nanowires, the UCI MRSEC team, consisting of the groups from BU and UCI, aims to understand their electronic structure and electron transfer mechanism. The team is systematically developing a protocol to combine:

i. Classical molecular dynamics (MD) to obtain thermally-averaged solvated nuclear positions
ii. All-atom first-principles density functional theory (DFT) calculation of the electronic structure
iii. Conductivity models associated with electron transfer mechanisms

For solvated ACC-Hex, recently synthesized by the UCI group (Hochbaum) with demonstrated efficient conductivity

- From all-atom DFT simulations including an explicit solvation shell (Figure 1 a), the team demonstrates that the near-gap orbitals span ACC-Hex and are nearly-degenerate (Figure 1 b-d).
- Considering structural fluctuations due to finite temperature, the team shows that there is a dynamic path for conductivity.
- These calculations provide a basis for incorporating DFT input into previously established conductivity models for biological systems

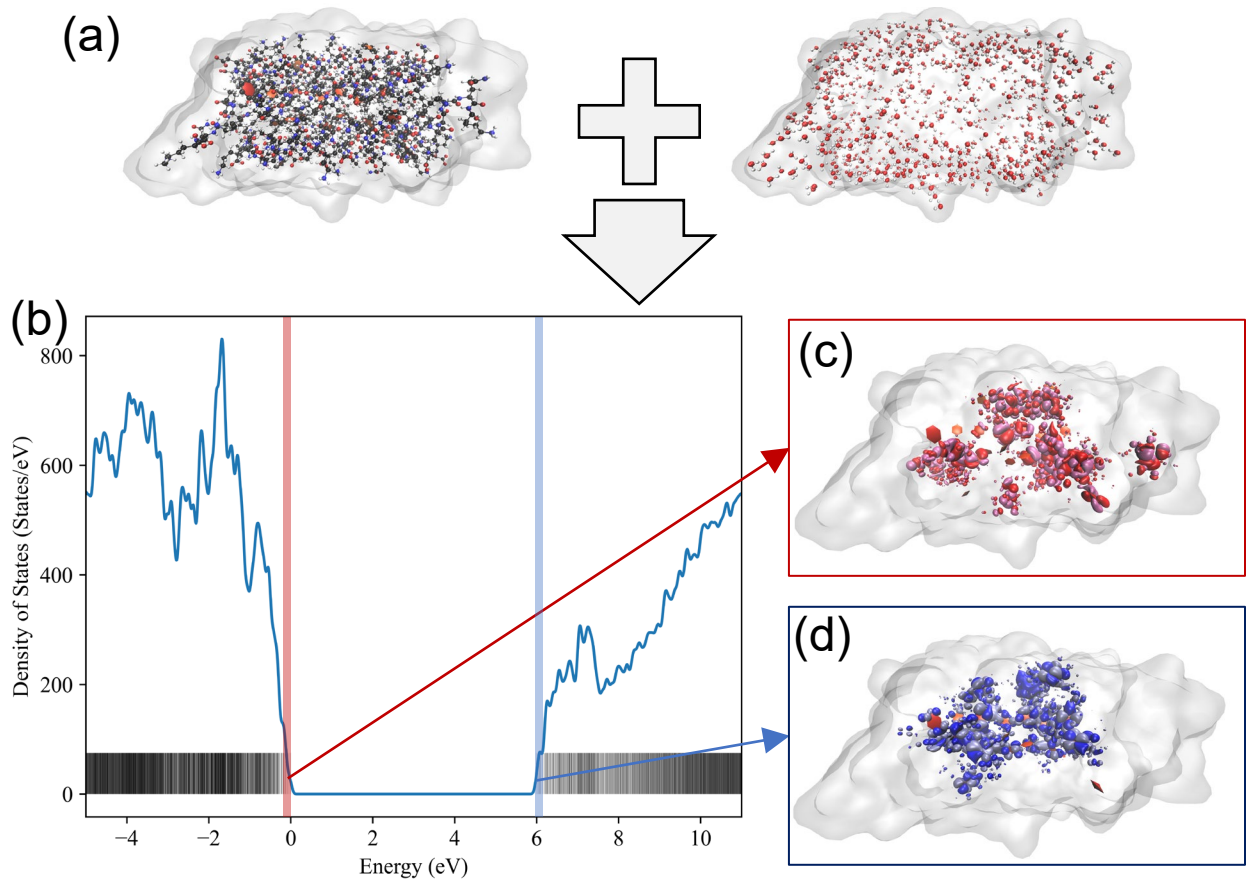

Figure 1: (a) All-atom simulations of ACC-Hex (left) with solvation shell (right). (b) DFT-predicted density of states near the gap. (c,d) Average density associated with near-gap orbitals, providing a path for conductivity.

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