Breakthrough in Molecular Electronics: Analytical Model Matches Experiments

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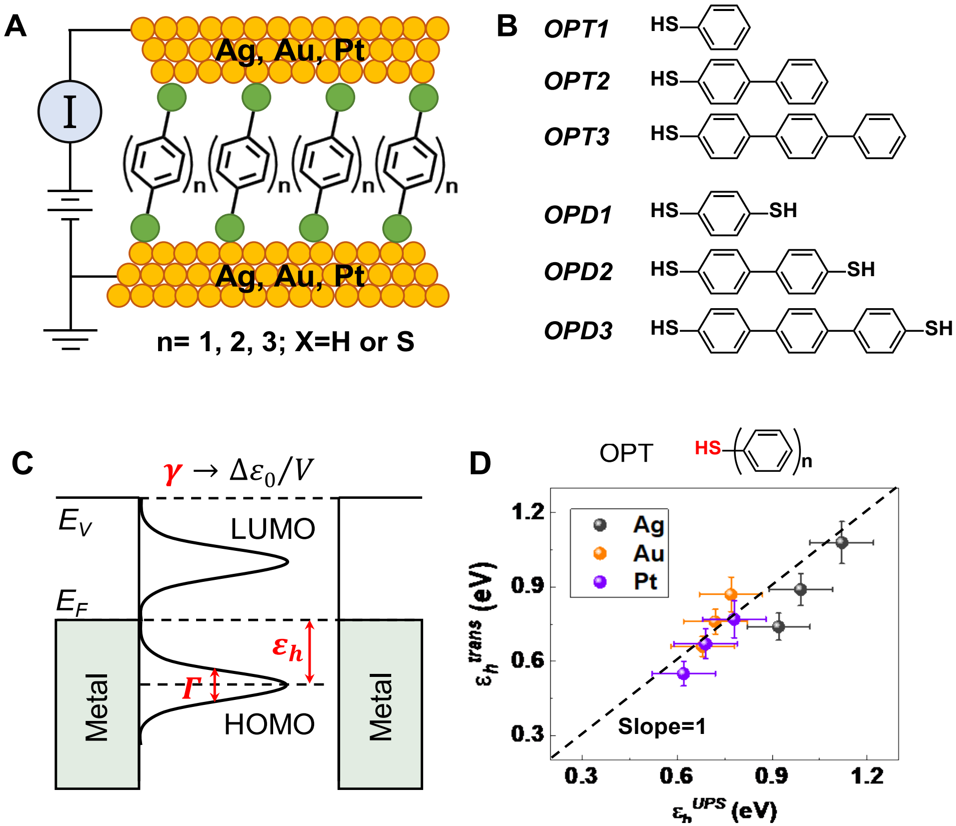

Figure 1.

A. Scheme of a molecular junction in which molecules are contacted by Ag, Au, or Pt metal electrodes.

B. Structures of pi-conjugated molecules used in this study.

C. Scheme of the junction electronic structure showing the definitions of key parameters, ε_h and Γ. characteristics.

D. Main result showing that ε_h determined by analysis of I-V characteristics (y-axis) matches ε_h independently determined by ultraviolet photoelectron spectroscopy (UPS; x-axis).

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Project Outcome: A “Single Level Model” equation is derived to describe the electrical conductance of pi-conjugated molecules. The equation allows key electronic structure properties to be extracted, such as ε_h, the offset of the molecular HOMO from the Fermi level, and Γ, the broadening of the HOMO due to coupling with the metal electrodes, Figure 1C. It is important to note that independent measurements of ε_h by ultraviolet photoelectron spectroscopy (UPS) agreed with ε_h extracted from conductance using the Single Level Model, Figure 1D. The results validate the model for quantitative analysis of molecular conductance.

Impact & Benefits: Electrical characterization of molecules connected between metal electrodes, Figure 1A, is a central focus of the field of molecular electronics. It is important both for potential applications of molecules in electronic devices and for a basic understanding of molecular conduction. A key roadblock in the field has been the lack of a simple quantitative model for describing molecular conductance. Under this award, the PI and his collaborators have proposed such a model and are demonstrating that it applies well to a wide variety of molecular junctions. The project promises further advancements in understanding and applications in molecular electronics.

Background & Explanation: This award is supported by the Macromolecular, Supramolecular, and Nanochemistry (MSN) program of the Division of Chemistry at NSF. The project funds research to understand the electrical conduction properties of molecules that may lead to new technology. The project also provides training for graduate students on a range of topics in chemistry including molecular synthesis, surface characterization, electrical measurements, and theoretical modeling. The work described here is published: Zuoti Xie, Ioan Baldea and C. Daniel Frisbie. *J. Am. Chem. Soc.* **2019**, *141*, 8, 3670-3681. DOI: 10.1021/jacs.8b13370