Estimation of π-π Electronic Couplings from Current Measurements

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Résumé en anglais	The - interactions between organic molecules are among the most important parameters for optimizing the transport and optical properties of organic transistors, light-emitting diodes, and (bio-)molecular devices. Despite substantial theoretical progress, direct experimental measurement of the - electronic coupling energy parameter t has remained an old challenge due to molecular structural variability and the large number of parameters that affect charge transport. Here, we propose a study of - interactions from electrochemical and current measurements on a large array of ferrocene-thiolated gold nanocrystals. We confirm the theoretical prediction that t can be assessed from a statistical analysis of current histograms. The extracted value of t ≈ 35 meV is in the expected range based on our density functional theory analysis. Furthermore, the t distribution is not necessarily Gaussian and could be used as an ultrasensitive technique to assess intermolecular distance fluctuation at the sub-angstrom level. The present work establishes a direct bridge between quantum chemistry, electrochemistry, organic electronics, and mesoscopic physics, all of which were used to discuss results and perspectives in a quantitative manner.
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