PÔSTER - RESUMO - MATERIAIS E BIOMATERIAIS

SINGLE-ENZYME CONDUCTANCE CHANNELS INTEGRATED INTO INTERFACE-ENGINEERED HYBRID PLATFORMS FOR MOLECULAR BIOELECTRONICS

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Understanding and controlling charge transport at the molecular level is essential for advancing bioelectronics and developing devices inspired by biological systems. In this work, we investigated the electronic behavior of a single enzyme using scanning tunneling microscopy (STM)–based molecular junctions. A hybrid HOPG/DZS platform was rationally engineered to establish a direct relationship between conformational dynamics and electron transport, enabling the measurement of discrete conductance states of an individual enzymatic entity under well-defined electrode–molecule coupling conditions. Single-molecule measurements revealed multiple conductance states associated with dynamically accessed conformations of the enzyme. Transport analysis indicates that charge transfer occurs predominantly in the tunneling regime, where conductance is governed by quantum-mechanical transmission through the molecular energy landscape. Within the Landauer framework, conductance is determined by the transmission function, which depends

critically on the electronic coupling (G) between the molecular orbitals and the electrodes. Conformational rearrangements modulate G and the alignment of frontier orbitals relative to the electrode Fermi level, thereby altering transmission probability. The observed conductance behavior is consistent with a transport mechanism dominated by coherent tunneling rather than thermally activated hopping, as evidenced by the discrete and reproducible conductance states characteristic of phase-coherent electron transmission across the molecular junction. These findings demonstrate that the enzyme does not behave as a static electronic element, but rather as a dynamic quantum system in which structural flexibility directly regulates electron transmission pathways. To enhance stability, reproducibility, and charge injection efficiency, the enzyme was integrated into a molecule–solid hybrid interface designed to control molecular orientation, optimize electrode–molecule contact, and reduce structural heterogeneity. Morphological, spectroscopic, and electrical characterizations confirmed that interfacial engineering significantly influences electronic coupling strength and transport efficiency. Rational tuning of the interface enabled controlled modulation of conductance by stabilizing specific conformational states and optimizing G, demonstrating that charge transport arises from the interplay between intrinsic conformational dynamics and extrinsic interfacial design. This study establishes a unified framework that integrates single-molecule quantum transport physics with rational interface engineering, demonstrating that enzymatic systems can function as active quantum electronic elements when appropriately coupled to hybrid architectures.

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