The University of Texas at San Antonio

UTSA Physics and Astronomy

Friday, April 19, 2024 at 11:00 AM, AET 0.204

Enantiospecific Electron Transport in Chiral-Modified Molecular Junctions

Dr. Ignacio L. Garzón

Instituto de Física, Universidad Nacional Autónoma de México, Mexico City

Chirality is a geometric property of matter that can be present at different scales, especially at the nanoscale. Here, we investigate the manifestation of chirality in electron transport through a molecular junction. Spinless electronic transport through a pristine molecular junction is not enantiospecific. However, when a chiral metal cluster, C3-Au34, is attached to the source electrode, a different response is obtained in spinless electron transport between R and L systems: this indicates the crucial role of chiral clusters in triggering enantiospecific spinless electron transport.[1] In contrast, when an achiral metal cluster, C3v-Au34, is attached, no change in conductance occurs between enantiomeric systems. Using the Non-Equilibrium Green's Function method, we characterized this phenomenon by calculating the transmission and conductance of spin-unpolarized electrons. Our theoretical results highlight the importance of metal clusters with specific sizes and chiral structures in electron transport and support previously published experimental results that exhibited enantiospecific scanning tunneling measurements with intrinsically chiral tips.

[1] Omar Hernández-Montes, Ignacio L. Garzón, and J. Eduardo Barrios-Vargas
"A chiral metal cluster triggers enantiospecific electronic transport"
Phys. Chem. Chem. Phys. (2024) DOI: 10.1039/d3cp04581a

Ignacio L. Garzón is Professor of Physics at the Universidad Nacional Autónoma de México. He is recognized as one of the leading theoreticians in Mexico in the field of physicochemical properties of nanomaterials. His area of research includes theoretical-computational studies on the shape and morphology of bare and ligand-protected metal clusters and nanoparticles to predict and understand their electronic, optical, and other physical and chemical properties. He has published over 100 scientific papers, many of them in high-impact journals such as Chemical Society Reviews, Accounts in Chemical Research, Nature Communications, Small, Nano Letters, Journal of the American Chemical Society, and Physical Review Letters, among others. He has been cited more than 6150 times, and his *h*-index is 42, according to Google Scholar data. His main scientific contributions are related to studies on the structural and vibrational properties and the chirality of bare and ligand-protected metal clusters. Prof. Garzón is a member of the Mexican Academy of Sciences.

Faculty Host: Dr. Xochitl Lopez-Lozano