Covalent Control of Excitonic Interactions: The Twist!

Scientific Achievement

A CINT User Team demonstrated that molecular twist angles, not separation distance, control how efficiently energy moves between molecules. Chemical bonds that hold molecules in symmetric arrangements create uniform, efficient charge transfer. Without these bonds, molecules twist asymmetrically, creating diverse electronic behaviors useful for different applications.

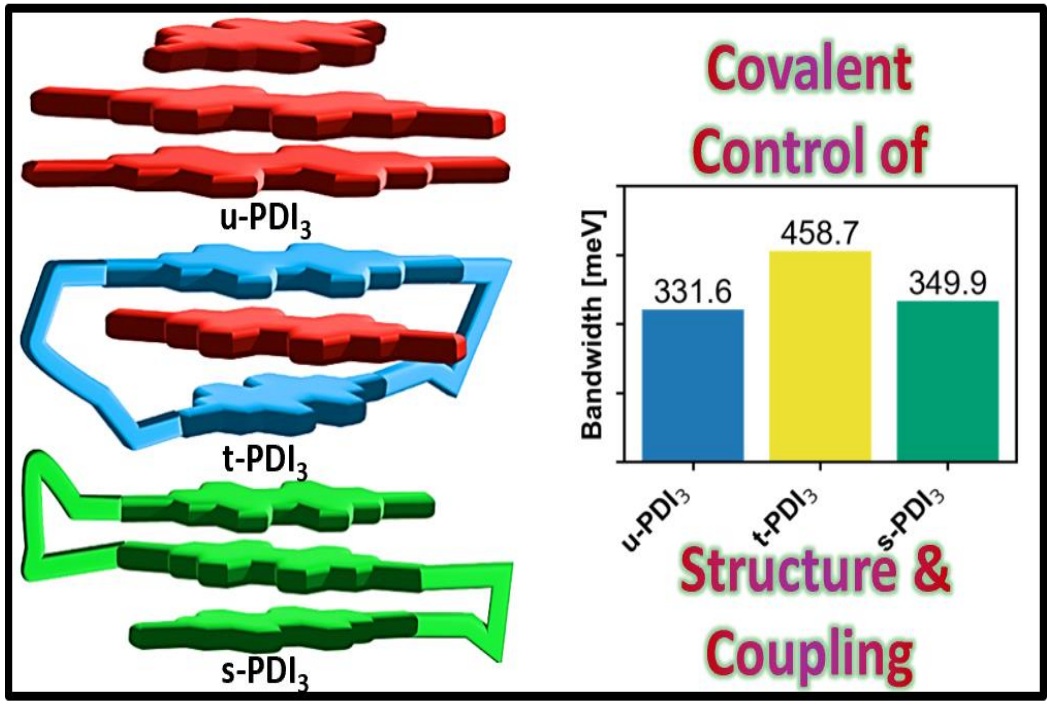

Figure: Molecular **twist** patterns provides design rules for building better organic solar cells and electronic devices.

Significance and Impact

Provides design guidelines for creating better solar cells, organic electronics, and light-harvesting materials. By controlling molecular geometry through chemical bonds, researchers can engineer materials with specific properties for energy conversion, flexible electronics, and advanced photonic devices.

Research Details

- Used *ab-initio* methods to predict electronic properties and energy transfer in three different PDI architectures
- Analyzed how molecular geometry, particularly twist angles and alignments, affects energy and charge movement
- Compared molecules without chemical bonds to those held together by different bonding strategies in water-like environments

Work was performed, in part, at the Center for Integrated Nanotechnologies.

Khanna, A.; Olivier, J.-H.; Fernandez-Alberti, S.; Tretiak, S. Covalent Control of Excitonic Interactions in Perylenediimide Trimers: A Computational Study. *Nano Letters.* 2026.