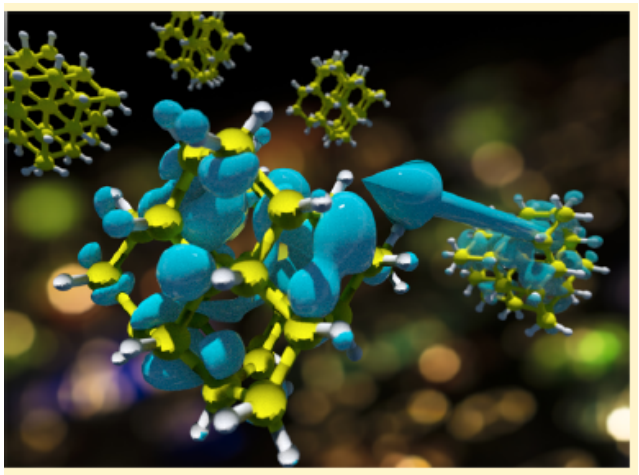
CHiMaD | Center for Hierarchical Materials Design
chimad.northwestern.edu

Charge Transport in Nanostructured Materials: Implementation and Verification of Constrained Density Functional Theory.

Matthew Goldey, Nicholas Brawand, , Márton Vörös, and Giulia Galli.



Caption: *Representation (blue isosurfaces) of charge transferred between different molecular building blocks. Calculations were performed with Constrained DFT.*

Scientific Achievement

Implementation and verification of a first principles code to compute charge transport, which we then used for hopping transport in OPV materials.

Significance

Development of a general capability to stud, from first principles, hopping transport.

Citation

Charge Transport in Nanostructured Materials: Implementation and Verification of Constrained Density Functional Theory, Matthew Goldey, Nicholas Brawand, Márton Vörös, and Giulia Galli, J. Chem. Theory Comput. 13 (6), pp 2581-2590 (2017).