Electron Transfer From Isolated Molecules To Biomolecules Part 1 Advances In Chemical Physics

#electron transfer #biomolecules #chemical physics #molecular electron transfer #isolated molecules

Explore the fundamental processes of electron transfer as it occurs from isolated molecules to complex biomolecules in this insightful Part 1 installment from Advances in Chemical Physics. This article delves into the intricate mechanisms governing these crucial interactions, providing a deep understanding of molecular and biological systems and their energy dynamics.

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Introduction
Oxidative phosphorylation
Catabolism
Oxidation and Reduction
Example
Change in Free Energy
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Threedimensional shapes of molecules
Trigonal shapes of molecules
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The Electron Transport Chain

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Ion Interaction
Ion Definition
Dipole Definition
IonDipole Definition
IonDipole Example
DipoleDipole Example
Hydrogen Bond
London Dispersion Force
Intermolecular Forces Strength
Magnesium Oxide
KCl
Methane
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Character of Triplet states Attachment/Detachment Plots
Derivative Coupling Input Code
Application #2: Closs Systems The equitorial-equitorial bridge
Real Time Ab-Initio Dynamics for the Closs systems (Brian Landry)
Diabatic Populations
And...the derivative couplings confirm that the EET goes through a conical intersection
Graphical Proof: Plot diabatic derivative couplings
Conclusions (Part 2)
Final Conclusions: Take-Home Messages The basic functionality for analyzing electronic relaxation (including electron and energy flow is now in Q-Chem)
What is triplet energy transfer?
Conclusions (Part 1) Derivative Couplings are available in Q-Chem between excited states at the CIS/TD-DFT level . We can work beyond TDA (with TDHF or RPA)
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The domain of quantum mechanics
Key concepts in quantum mechanics
Review of complex numbers
Complex numbers examples
Probability in quantum mechanics
Probability distributions and their properties
Variance and standard deviation
Probability normalization and wave function
Position, velocity, momentum, and operators
An introduction to the uncertainty principle
Key concepts of quantum mechanics, revisited
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In the Bohr model of the atom, electrons circle the nucleus in the same way that planets orbit the sun.
Maximum number of electrons = 2n?
Within each energy level are sublevels. The sublevels are labeled s, p, d, and f. You need to memorize these 4 sublevels.
Within each sublevel, there are orbitals. This is the final location where electrons reside.
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FTL Action at Distance
How to Exploit?
Idea 1: Repeat Measurements
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Where From Here?
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Nitrate Ion No3 Minus
Lone Pairs
Lone Pairs Repel More Strongly than Bonding Pairs
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Water
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Entropy
Entropy Analogy
Entropic Influence
Absolute Zero
Entropies
Gibbs Free Energy
Change in Gibbs Free Energy
Micelles
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Order of magnitude
Two equations: Large vs small
Stoke-Einstein (Large)
When use which equation
Wilke-Chang (small)
Viscosity of solution! (T and C)
Short summary of mass transfer
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Knowing the change in velocity, you can make predictions
Buoyant Force
About 1 Newton
Newton's Law of Universal Gravitation
Energy and thermodynamics
Energy is not a vector
20 mph (32 km/h) faster almost doubles the energy of a car
Total energy is kinetic plus potential
Gasoline has chemical potential energy
Thermodynamic Systems Thermal Energy
Kinetic energy of car converted to thermal energy from friction of the brakes
Entropy is a measure of "disorder," or the information required to describe microstates
2nd law of thermodynamics: Entropy of an isolated system can never decrease
Gasoline more useful for work than heat from exhaust
Exhaust will not rearrange itself to become gasoline
but gasoline can be converted to heat and exhaust
One way flow of entropy appears to be the only reason there is a forward flow of time
Electromagnetism: Study of interaction between electrically charged particles
Moving charges create magnetic fields
Moving magnetic field affects charges
Magnets always have two poles
Faraday's law
Moving magnetic field creates an electrical field
Laws of physics on moving train is same as laws of physics standing still
Energy is not continuous, but is quantized
Heisenberg's Uncertainty Principle uncertainty in momentum
Note: central cluster of electrons exaggerated for illustration. Only a probability cloud exists
Model of hydrogen atom with electron at lowest energy state
A quantum system can be elementary particles
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Disaccharides
Polysaccharides
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KCl
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Gibbs Free Energy
Change in Gibbs Free Energy
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Total energy is kinetic plus potential
Gasoline has chemical potential energy
Thermodynamic Systems Thermal Energy
Kinetic energy of car converted to thermal energy from friction of the brakes
Entropy is a measure of "disorder," or the information required to describe microstates
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Gasoline more useful for work than heat from exhaust
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Electromagnetism: Study of interaction between electrically charged particles
Moving charges create magnetic fields
Moving magnetic field affects charges
Magnets always have two poles
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A quantum system can be elementary particles
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