

Beyond Scalar Measures: Directional Chemical Perspective with Next Generation QTAIM

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The theoretical chemical physics/bio-chemistry that the BEACON research group undertakes seeks to develop new theory and explanations for chemical observations whilst also posing questions to be answered by future experiments. Our (next generation) QTAIM based research pioneers new theoretical tools that provide a new 3-D vector based perspective to solve what was only until recently considered unsolvable. An example of this was our explanation of chirality using only chemical measures [1]. By providing new tools based on ignoring previous assumptions in theoretical chemistry/chemical physics we can currently address new areas such as isotope separation, excited state dynamics [2], prediction of competitive and non-competitive ring-opening reactions [3], excited state phenomena [4], physical properties including the application of E-fields [5] and spectroscopic response.

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[1] Chirality-Helicity Equivalence in the S and R Stereoisomers: A Theoretical Insight, *Journal of the American Chemical Society*, **141**(13), 5497–5503 (2019). DOI: 10.1021/jacs.9b00823.

[2] QTAIM and Stress Tensor Characterization of Intramolecular Interactions Along Dynamics Trajectories of a Light-Driven Rotary Molecular Motor, *J. Phys. Chem. A* **121**(25), 4778–4792, (2017). DOI: 10.1021/acs.jpca.7b02347.

[3] A vector-based representation of the chemical bond for predicting competitive and noncompetitive torquoselectivity of thermal ring-opening reactions, *International Journal of Quantum Chemistry* **118**(20), e25707 (2018). DOI:10.1002/qua.25707

[4] A 3-D Bonding Perspective of the Factors Influencing the Relative Stability of the S_1/S_0 Conical Intersections of the Penta-2,4-dieniminium Cation (PSB_3), *International Journal of Quantum Chemistry*, **119**(11), e25903 (2019). DOI: 10.1002/qua.25903

[5] The Destabilization of Hydrogen-bonds in an External E-Field for Improved Switch Performance, *Journal of Computational Chemistry*, Early View (2019). DOI: 10.1002/jcc.25843



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