Beyond Scalar Measures: Directional Chemical Perspective
with Next Generation QTAIM

Samantha Jenkins

Key Laboratory of Chemical Biology and Traditional Chinese Medicine Research and Key Laboratory of Resource National and Local Joint Engineering Laboratory for New Petro-chemical Materials and Fine Utilization of Resources, College of Chemistry and Chemical Engineering, Hunan Normal University, Changsha, Hunan 410081, China

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.

samanthajsuman@gmail.com

http://www.beaconresearch.org


Ph.D. at Salford University in 2000, Associate Professor (Docent in Chemical Physics) University West 2006, Professor Chemistry, (2010) College of Chemistry and Chemical Engineering, Hunan Normal University, Director of Theoretical and Computational Chemistry.