YNU 横浜国立大学
YOKOHAMA National University

物理工学談話会　4月27日（月）午後 13：30〜

会場：総合研究棟W701　世話人：レービガー　ハンネス

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Beyond Energetic and Scalar measures: Next Generation QTAIM

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Next Generation Quantum Theory of Atoms in Molecules (NG-QTAIM) is currently the only vector-based quantum chemical theory as all other quantum chemical theories are scalar-based. NG-QTAIM can, for instance, be used to distinguish enantiomers, isotopomers undergoing normal modes of vibration, predict ring-opening reaction products, ground and excited states at a conical intersection and predict reaction pathways of permutation-inversion isomers. As a consequence, NG-QTAIM can uniquely be used to investigate iso-energetic phenomena where the reliance on differences in geometric measures is removed.

Biography:Professor Dr. Samantha Jenkins,
professor of Chemistry at Hunan Normal University, Changsha, China, she joined the Hunan 100 Talents Project in 2010. Research interests: Developing the theory of atoms in molecules (QTAIM) to form Next generation QTAIM. She has a track record of research funding in Sweden and China with the National Natural Science Foundation of China (NSFC), has published in high impact journals including the Journal of the American Chemical Society (JACS), an invited perspective article on her research in WiRES: Computational Molecular Science and has a book for Springer/Nature on her researchdue to be published on the subject in April 2023. In 2013 she won a Chinese Government Friendship Award and in 2021 received the Hunan International Science and Technology Cooperation First Class Award.