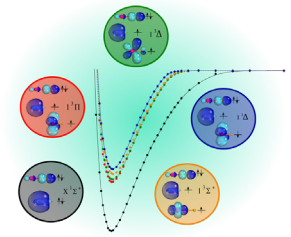
The research in our group focuses upon the development and understanding of computational methodologies, and studies in transition metals and heavy element chemistry, catalysis, protein modeling, drug design/understanding of disease, environmental/green chemistry, and many other areas. One of the great features of theoretical and computational chemistry is that they can be utilized to investigate a broad array of challenges, and our group is engaged in areas including quantum mechanical and quantum dynamical method development, thermochemical and spectroscopic studies of small molecules, protein modeling and drug design, catalysis design, environmental challenges (i.e., CO_2, PFAS), heavy element and transition metal chemistry, and mechanical properties of materials.

Development and understanding of methodologies – Much of our group's efforts are focused upon the development of ab initio approaches that aim for accurate prediction of thermochemical properties across the periodic table. Included in our efforts has been the development of successful and versatile ab initio composite schemes, called correlation consistent Composite Approaches (ccCA), that provide reduced computational cost (in terms of computer time, memory, and disk space) means to achieve energetic predictions. The approaches are useful for ground-state, excited-state, and transition- state energies, and can be applied to situations where single-reference wavefunctions or where multireference wavefunctions (i.e., bond-breaking, diradicals) are necessary. Included in our work is the development of Gaussian basis sets, providing new additions to the correlation consistent basis set family, and rigorous evaluation of existing and new basis sets. Another area of interest is in gauging the performance of methodologies, such as density functional theory, particularly for situations where there may be few, if any, needed experiments for comparison. Efforts extend across the periodic table, with substantial focus upon the transition metals.

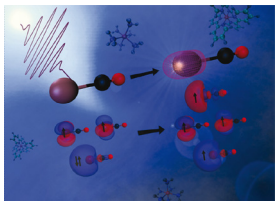
This paper focused upon design strategies for the prediction of pKa of transition metal species. (From J. Comp. Chem. 2020, 41, 171, cover article.)

Heavy element chemistry – The complexity of the heavy elements results in their great utility in applications from cell phones to stealth technology. We are developing a better understanding of the fundamental properties of heavy element species, as well as the methodologies needed to describe their energetic and spectroscopic properties, and utilizing this knowledge in areas such as separation science and the development of new methodologies for heavy elements.



An analysis of the ground and excited state potential energy channels for LuF. (J. Chem. Phys. 2021.)

Quantum dynamics – A part of our group's efforts focuses on time-dependent quantum mechanical approaches across the periodic table. Of particular interest in addition to our development of methodologies is the study of light-driven phenomena.



The spin density difference and the participating orbitals in a light-induced spin flip in FeCO determined using a newly developed time-dependent spin-orbit coupling configuration approach from our group, designed to describe quantum dynamical phenomena. (From Phys. Chem. Chem. Phys. 2019, 21, 7265; back cover article.)

Catalysis – Homogeneous and heterogeneous catalysis are of interest, and we investigate a broad range of catalytic reactions, including novel electrocatalysts.

Drug design/understanding disease and biological function – We utilize a variety of computational chemistry approaches towards the understanding and design of potential pharmaceuticals for diseases including cancers and tuberculosis. We also investigate structure activity relationships, the role of signal transduction cascades in disease, and approaches to modulate biological functions.

Environmental and sustainable chemistry – We investigate the impact at the molecular level of contaminants such as CO_2 and PFAS compounds. For PFAS, the impact of the compounds on human and animal proteins and their absorption and transport in soil and water are of focus. Routes for possible mitigation are also considered.

Per- and Polyfluoroalkyl Substances (PFAS) are prevalent in day-to-day products. Here, the interaction of some of the most prevalent PFAS with peroxisome proliferator-activated receptor gamma (PPARγ), a nuclear receptor fundamental to the regulation of genes is considered. (ACS Omega, 2021)

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517-353-1111

Selected Publications

Coupled Electron and Nuclear Motion in Strong Laser Fields, L.E. Aebersold, I.S. Ulusoy, and A.K. Wilson, *Phys. Rev. A* **2019**, *100*, 023406.

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Domain-Based Local Pair Natural Orbital Methods within the correlation consistent Composite Approach, P. Patel and A.K. Wilson, *Journal of Comp. Chem.* **2020**, *41*, 800-831.

Binding of Per- and Polyfluoroalkyl Substances to Human Pregnane X Receptor, T. Lai, Y. Eken, A.K. Wilson, *J. Comp. Chem.* **2020**, *54*, 15986.

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SAMPL7 Host-Guest Binding Prediction by Molecular Dynamics and Quantum Mechanics, Y. Eken, N.M.S. Almeida, C. Wang, A.K. Wilson, *J. Comp.-Aided Mol. Des.* **2021**, *35*, 63-67.

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