

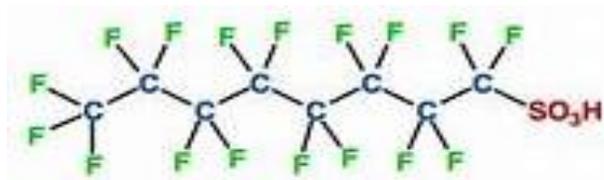
Sustainable Chemistry in the Angela Wilson Research Group

Computational chemistry applications and development to address:

Per- and polyfluoroalkyl Substances (PFAS)

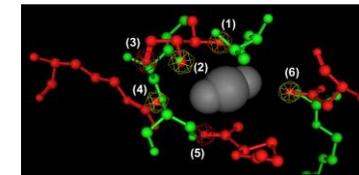
- “zombie” chemicals or “forever chemicals”
- > 4,000 molecules
- Found in many non-stick and water-proof coatings (e.g., Teflon cookware), food packaging, stain repellants (e.g., Scotchguard), fire-fighting foams, . . .
- Impact and mitigation strategies; health concerns

Quantum mechanics, protein modeling

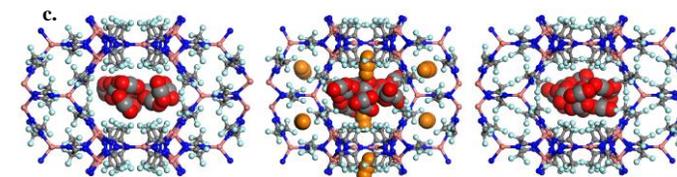


CO₂ mitigation

- Sequestration, utilization
- CO₂ binding sites in proteins
- Scrubbers
- Reverse water-gas shift reactions (homogenous and heterogenous catalysis)



Quantum mechanics, Monte Carlo, molecular dynamics



Fuels to value-added chemicals

- Feedstocks
- Kinetics, thermodynamics

Quantum mechanics, quantum dynamics



REU participant selects from these projects, or from other group projects on transition metal catalysts or heavy element chemistry.

Wilson research group, September 2019.