Reactivity of silyl ketenes and gas adsorption to Buckybowls

selected examples of undergraduate research in computational chemistry

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This poster presents selected examples from research in our lab.

Reactivity of silyl ketenes:[1] Silyl ketenes feature a rich reactivity owing to their bifunctionality embodied by the ketene function, C=C=O. Oligomerization along these functions has been proposed as a route to create products with potentially desirable properties, such as degradability. However, the C=C vs. C=O reactivity needs to be understood to specifically target a desired product. This work utilizes contemporary density functional theory in combination with semiempirical quantum approaches to investigate the reactivity of silyl ketenes with representative nucleophiles in order to rationalize reactivity trends.

Gas adsorption to Buckybowls:[2] Buckybowls are bowl-shaped (geodesic) molecules that can bind small gaseous molecules. Adsorbate binding is enhanced by the curvature of the Buckybowl. Inspired by this insight, this work utilizes density functional theory to investigate impacts of Buckybowl structure on the binding of gaseous molecules in order to identify trends and suggest potential modifications to enhance adsorbate binding.

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