CHEMISTRY DEPARTMENT ORAL PRESENTATIONS

Presenter	Title	Description	MCLT	Start -End	Day
Sean Murphy	Porous Carbon as Scaffolding for Iron-air Electrodes	Metal-air batteries exhibit promising energy storage for future applications in electronics and electric car industries, but currently do not provide enough power for practical use. Our electrode was created by using a macroporous carbon scaffold for iron oxide that was deposited from a 25-mM potassium ferrate solution. We hypothesized that an increase in surface area would allow more electrochemical reactions to occur, resulting in a higher power output. The iron-air electrodes can provide a power of up to 360±12 W kg-1 of FeOx, discharged at 2 A, and are capable of discharging at 10 A for 20 s. With an average energy of 155±37 Wh kg-1 of FeOx, this is less than half of the energy of zinc-oxide batteries currently in production. Our electrodes do not account for the entire mass of a battery, which means the power and energy values are even lower than the current data suggests in comparison to batteries. This means we are not accessing as much of the FeOx as we originally intended. The samples also lose >50% of their electrochemical capacity after 10 cycles; due to either the loss of electrode mass during cycling, or an altered surface morphology which could reduce redox activity.	103	1:10 -1:50 PM	F
Drew Huff	In-silico Screening of Highly Functionalized Benzofulvenes as Competitive Inhibitors of Human Thioredoxin Reductase 1	The goal of our work is to explore several small molecules as possible inhibitors of Human Thioredoxin Reductase 1 (TrxR1). TrxR1 inhibition has been shown to induce tumor cell apoptosis and prevent metastasis. We aim to develop a library of compound leads and better understand the chemical nature of the protein-ligand docking interaction for the future development of potential therapeutics against TrxR1. Computational modeling with AutoDock Vina was employed to determine the docking affinity potential of a series of fulvene-based small molecule ligands. The structural activity relationships of highly functionalized benzofulvene compounds revealed several ligands with excellent in-silico affinity, a few examples have even produced nanomolar binding affinity. Current work has transitioned into producing a full synthetic library and in-vitro testing.	103	1:50 -2:30 PM	F