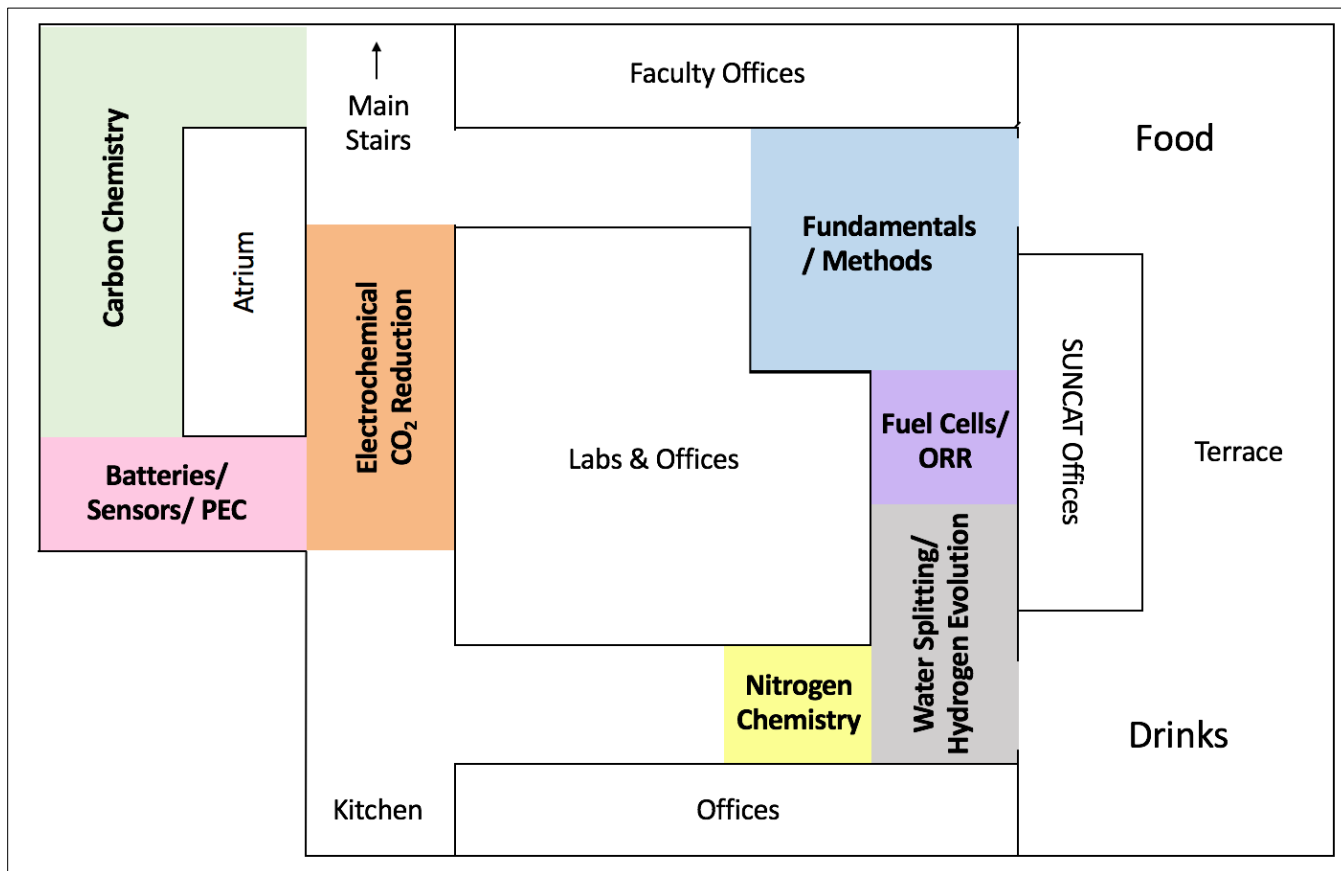


# SUNCAT Summer Institute 2017 Poster Sessions

Shriram Center, third floor by the terrace and blue atrium

Monday and Tuesday (August 14&15), 7:30-9:30 pm



**Monday, Session 1: 7:30pm – 8:30pm**

	<b>First Name</b>	<b>Last Name</b>	<b>Title</b>
Batteries	Shuting	Feng	Design of stable organic electrolytes for Li-O2 batteries
	Graham	Leverick	The Role of Iodide on the Formation of Lithium Hydroxide in Lithium-O2 Batteries
	Thomas	Østergaard	Oxidation of Ethylene Carbonate in Li-ion Batteries
Carbon Chemistry	Karthik	Akkiraju	Reaction Pathways for Formaldehyde Oxidation on Manganese Oxide Catalyst
	Qiyuan	Fan	Theoretical study of n-butane hydrogenolysis on metal surfaces
	Pushkar	Ghanekar	Metal oxide interfaces for Water Gas Shift Reaction: Mechanistic understanding at Pt/MgO interfaces
	Xiao	Li	First-principles investigation of the active site and the reaction mechanism of acetaldehyde hydrodeoxygenation over Ru/TiO2
	Christopher	Riley	Nickel-Doped Ceria for Selective Acetylene Hydrogenation
	Max	Schumann	Catalytic synthesis of higher alcohols from synthesis gas over Rh based catalysts
	Luca	Silvioli	Electrocatalytic conversion of propene
	Hari	Thirumalai	A Screening Study of Methane Activation on Metal Exchanged Zeolites Based on Uncertainty Quantification
	Anna	Winiwarter	Electrochemical Oxidation of Hydrocarbons
Electrochemical CO <sub>2</sub> Reduction	Denghui	Xing	Hydrogenation of Acetylene by Graphdiyne-Supported Triatomic Clusters: A Size Mismatch Effect
	Alexander	Bagger	Electrochemical CO2 reduction on metals and porphyrine-like structures
	Divya	Bohra	Rational design of carbon dioxide electroreduction catalysts using multiscale modeling
	Meredith	Fields	Phosphides and Sulfides: Applications in Electrocatalysis
	Kai	Liu	Au-Cu bimetallic thin film for CO2 reduction
Fuel Cells, ORR	Jakob Ejler	Sørensen	Reactivity of Copper Nanoparticles for CO2RR
	Logi	Arnarson	The electrolyte interface under ORR studied with DFT
	Olga	Vinogradova	Catalyst Activity at Fuel Cell Cathode for Oxygen Reduction
	Anders	Jensen	Exploring the oxygen reduction reaction of nanoporous catalyst in gas diffusion electrode
	Sung Beom	Cho	Transition metal-based catalysts on stable and corrosion-resistant supports for oxygen reduction reaction
Yanyan	Sun	Efficient electrochemical hydrogen peroxide production from molecular oxygen on nitrogen-doped mesoporous carbon catalysts	

Fundamentals, Methods	Ahmad	Gardizi	Transition state investigations - based on atomic scale simulation
	Maria	Escudero-Escribano	Electrochemical Interfaces for Sustainable Energy
	Thomas	Maagaard	Combining UHV-STM and electrochemistry for model studies of catalysts for ORR
	Lars	Blumenthal	On the use of atomistic and continuum solvation models for electronic energy level alignment
	Jonathan	Quinson	Unprotected precious metal nanoparticles for catalysis
	Kaspar	Holst-Olesen	Anion adsorption on NPMC-sites
	Niklas	Mørch Secher	2-Dimensional Materials as Substrate for Catalytically Reactive Centers
	Kasun	Gunasooriya	Modeling-Guided Design of Catalytic Processes
	Rickey	Terrell	Structural Characterization of Platinum Alloy Nanoparticles using Inorganic NMR
	Zeeshan	Ahmad	Quantification of uncertainty in first-principles predicted mechanical properties of solids
Nitrogen	Jaysree	Pan	Theoretical modelling of electrochemical ammonia evolution
	Juan	Gonzalez	Why Pt(111) does not represent a good model to simulate the ammonia combustion reaction over platinum?
Water Splitting, Hydrogen Evolution	Hyunho	Noh	Sub-Nanosized Metal Sulfide Clusters in Metal-Organic Frameworks for Electro- and Photo-Catalytic Hydrogen Evolution
	Jose Luis	Lima de Jesus Silva	Nanodevices as micro-reactors for studying electrocatalytic hydrogen evolution reaction
	Ben	Levy-Wendt	Catalytic Enhancement of Cobalt Disulfide Hydrogen Evolution Catalysts Using Gold Nanoparticles
	Dave	Palm	Activation and Stabilization of Chalcopyrite Light Absorbers for Photoelectrochemical Hydrogen Production
	Xinjian	Shi	Transition metal doped tungsten sulfide for hydrogen evolution

### Monday, Session 2: 8:30pm – 9:30pm

	First Name	Last Name	Title
Batteries, Sensors, PEC	Changhyeok	Choi	Ti(N5)4 as a Potential Nitrogen-Rich Stable High-Energy Density Material
	Noushin	Omidvar	Electrode-Electrolyte Interfaces Probed by Quantum-Chemical Simulations and Machine Learning for Lithium-Ion Batteries
	Larissa	Kunz	Photocatalytic Hydrogen Production Using Composites of Brookite Titania Nanorods and Carbon Nitride
Carbon Chemistry	Andrew	Rosen	DFT Study of Metal Oxide Nanoclusters for C-H Bond Activation
	Woonghyeon	Park	DFT study of CO oxidation on NiO <sub>1-x</sub> /Pt(111)
	Andrew	Riscoe	Converting Methane to Methanol with Nature Inspired Materials
	Jiamin	Wang	First-Principles Studies of CO Oxidation on MgAl <sub>2</sub> O <sub>4</sub> supported Iridium Single Atoms
	Wenqiang	Yang	Hydrodeoxygenation of Succinic acid to 1-4 Butanediol: A DFT study
	Diego	Gomez Gualdron	Framework-topology-dependent catalytic activity of metal-organic frameworks

	Huong	Dang	Activation and carbon formation in bi-reforming of methane
	Ebrahim	Tayyebi	DFT calculation of N <sub>2</sub> &Co <sub>2</sub> reduction on transition metal oxides and nitrides
	Moyahabo	Chuma	Computational study of methane oxidation over palladium oxide
Electrochemical CO <sub>2</sub> Reduction	Thomas	Hogg	CO <sub>2</sub> and CO Reduction on Mass-Selected Cu Nanoparticles
	Xingli	Wang	Tunable Selectivity of CuO <sub>x</sub> Nanoparticles on CO <sub>2</sub> /CO Electroreduction Reaction
	Yifan	Li	Evolution of Copper Nanostructures under CO <sub>2</sub> Electroreducing Conditions
	Matthew	Mayer	Overcoming barriers in electrochemical conversion of carbon dioxide
	Sheena	Louisia	Size-dependent structural changes of copper nanoparticles during CO <sub>2</sub> electrolysis
	Sunmoon	Yu	Silver nanoparticle ensembles for carbon dioxide electroreduction
Fuel Cells, ORR	Yashpal	Singh	Mechanism of ORR on metal doped borophane
	Weichao	Wang	Investigation of High Oxygen Reduction Reaction Catalytic Performance on Mn-based Mullite SmMn <sub>2</sub> O <sub>5</sub>
	Dilip	Krishnamurthy	Structure-Activity Descriptor for Electrocatalytic Activity of Nickel Sulfides for the Oxygen Reduction Reaction
	Seoin	Back	An Importance of Ligand Effects Breaking the Scaling Relation for Core-Shell Oxygen Reduction Catalysts
	Gurjyot	Sethi	Platinum Overlayer Catalysts for Oxygen Reduction Reaction
Fundamentals, Methods	Gregory	Houchins	Uncertainty Quantification for Predicting Magnetic States at the GGA Level
	Juhyung	Lim	Single atom catalysts on 2D material supports
	Siwen	Wang	Coordination-based Descriptors for Rational Design of Metal Nanocatalysts
	Xu	Huang	Extending Accurate DFT Modeling for the Study of Interface Reactivity and Environmental Applications
	Liheng	Wu	Accelerating Nanocatalyst Synthetic Development Using In Situ Small Angle X-ray Scattering
	Hanyu	Ma	Shape-controlled synthesis of palladium phosphide for catalytic hydrodesulfurization of refractory sulfur compounds
	Adarsh	Dave	Electrolyte Discovery Using High-Throughput Data-Driven Approaches
	Victor	Venturi	Uncertainty Quantification of Thermal Properties using First-Principles Computation
	Thomas	Batchelor	Catalysis on high entropy alloys
	Nihar	Jena	Design of electrocatalysts for sensor applications
	Hsin-Yi	Wang	In-situ observing the catalyst and surface reaction during the electrochemical catalysis

Nitrogen	Gray	Laughlin	Surface Coverage Effects on Ammonia Chemistry
	Bar	Mosevitzky	Catalytic pollutant abatement of urea ammonium nitrate fuel combustion effluent on platinum and ruthenium
	Chengshuang	Zhou	Metal Nitrides as Highly Efficient Electrocatalysts for Electrochemical Synthesis of Ammonia
Water Splitting, Hydrogen Evolution	Lauren	King	Transition Metal Arsenides for the HER
	Tiantian	Wu	DFT investigation of water splitting on ceria surface
	Vaidish	Sumaria	Quantification of Uncertainty in activity volcano relationships for Oxygen Evolution Reaction
	Sravan kumar	Kanchari bavajigari	On Identification of Labile Oxygen in Ceria-Based Solid Solutions: Which Oxygen Leaves the Lattice?
	Reshma	Rao	Exploring the pre-oxygen evolution surface chemistry on RuO <sub>2</sub> (110)

### Tuesday, Session 1: 7:30pm – 8:30pm

	First Name	Last Name	Title
Batteries, Sensors, PEC	Holden	Parks	2D Heterostructures as Novel Li-ion Battery Anode Materials
	Yang	Yu	Understanding the anion redox process in Li-ion battery cathode materials
	Hendrik	Heenen	The effect of occupational disorder on ion mobility in Li <sub>4</sub> Ti <sub>5</sub> O <sub>12</sub> battery materials
	Mohnish	Pandey	Chalcogenides as Light Absorbing Materials for Single Junction and Tandem Device
Carbon Chemistry	Zhenwei	Wu	Intermetallic compound catalysts for light alkane dehydrogenation
	E. Sebastian	Gutterød	CO <sub>2</sub> hydrogenation over Pt-containing UiO-67 Zr-MOFs - the base case
	Yunyun	Zhou	Highly porous carbon sheets supported Fe <sub>3</sub> O <sub>4</sub> nanoparticles for Fischer-Tropsch synthesis to light olefins
	Julia	Schumann	Catalysts for Higher Alcohol Synthesis
	Hassan	Aljama	Theoretical study on methane activation using alkaline metal oxides
	Allegra	Latimer	A Theoretical Study of Methanol Oxidation on RuO <sub>2</sub> : Bridging the Pressure Gap
	Jonathan	Snider	In-X bimetallic catalysts for selective CO <sub>2</sub> hydrogenation to methanol
	Joshua	Willis	Systematic Identification of Promoters for Methane Oxidation Catalysts by Using Size- and Composition-Controlled Pd-based Bimetallic Nanocrystals
Arvin	Kakekhani	Developing Schemes for Selective Partial Oxidation of Methane	

Electrochemical CO <sub>2</sub> Reduction	Feng	Jiao	Electrochemical Carbon Dioxide Conversion
	Charlotte	Kirk	CO Reduction on Metal Doped Graphene
	Andrew	Wong	Palladium Nanoclams for CO <sub>2</sub> Reduction for Coupling to Microbial Communities
	Lei	Wang	Electroreduction of carbon monoxide on polycrystalline copper
	Stephanie	Nitopi	Screening of Binary Alloy Thin Films for Electrochemical CO <sub>2</sub> /CO Reduction
Fuel Cells, ORR	Shouping	Chen	Atomic Migration in Pt-Ni Rhombic Dodecahedron under Annealing and its Effect on Oxygen Reduction Reaction (ORR) Activity
	Megha	Anand	2D materials for OOR activity
	Zhijia	Chen	Development of a reactor with carbon catalysts for modular-scale, low-cost electrochemical generation of H <sub>2</sub> O <sub>2</sub>
	Anjli	Patel	Metal-Doped Carbon Nitride Catalysts for the Oxygen Reduction Reaction
	Sara	Kelly	Transition Metal Oxides for Selective 2-electron Water Oxidation
Fundamentals, Methods	Søren	Scott	Dynamic effects in electrocatalysis
	Lide	Oar-Arteta	Metal Organic Framework Mediated Synthesis in Catalysis
	Svante	Hedström	Intramolecular Charge Transfer in Molecular Catalysts
	Denis	Kuznetsov	Tuning the metal redox transitions in oxides via inductive effect
	Jeppe	Kari	Application of the Sabatier principle in heterogeneous enzyme catalysis
	Xiaohong	Zhang	Molecular simulation study of how water affects free energy of adsorption in aqueous phase heterogeneous catalysis
	Joe	Gauthier	Challenges in Modeling the Electrochemical Interface with a Polarizable Continuum Model
	Vanessa	Bukas	The electrochemical interface under potential bias: Microscopic insights from first-principles
	Luke	Roling	Coordination-Based Model for Bimetallic Nanoparticles
	Zeeshan	Ahmad	Quantification of uncertainty in first-principles predicted mechanical properties of solids
Nitrogen	Suzanne	Andersen	Detection and quantification of electrochemically synthesized ammonia
	Fatemeh	Hanifpour	Electro-reduction of N <sub>2</sub> to ammonia at ambient conditions: from theory to experiment
	Jane	Mugo	Ammonia Oxidation : A DFT Study
Water Splitting, Hydrogen Evolution	Alaina	Strickler	Gold-Core Transition Metal Oxide-Shell Nanoparticle Electrocatalysts for Enhanced Oxygen Evolution
	Colin	Dickens	Oxygen Evolution Reaction: Electronic Structure to Kinetics
	Reuben	Britto	Molybdenum Disulfide as a Protection Layer and Catalyst for Solar Water Splitting Photocathodes
	Joel	Sanchez	Intercalated Ni and Fe within ZrP for the OER

**Tuesday, Session 2: 8:30-9:30 pm**

	<b>First Name</b>	<b>Last Name</b>	<b>Title</b>
Batteries, Sensors, PEC	Thaneer Malai	Narayanan	Semi-solid flow battery for grid-scale energy storage
	Estefanía	Garijo del Río	Computational screening of light absorbing materials for water splitting
	Amedeo	Agosti	PHOTOTRAIN - Entreprenuring dynamic self-organized interfaces in photocatalysis: a multidisciplinary training network converting light into products
	Nihar	Jena	Electrocatalytic effects of biomaterials for sensor applications
Carbon Chemistry	Marat	Orazov	Tandem Catalysis for Ethanol Synthesis from Syngas
	Pallavi	Bothra	Effect of Promoters on Higher Alcohol Synthesis
	Amber	Janda	Sulfur-decorated rhodium catalysts for C2 oxygenate synthesis from syngas
	Emmett	Goodman	Monodisperse Pt/Pd Bimetallic Nanocrystals Demonstrate Platinum Effect on Palladium Methane Combustion Activity and Stability
	Eduardo	Valle	Modification of MoP catalyst for higher alcohol synthesis from syngas
	Jiang	Li	Electrochemical Oxidation of Methane on Sr <sub>2</sub> FeMoO <sub>6-δ</sub> (001) Surface at the Anode of Solid Oxide Fuel Cell from the Insight of First Principles
	Ang	Cao	Mechanism of Higher Alcohol Synthesis from Syngas on CuCo alloy
	Cody	Wrasman	Selective Oxidation of Methane to Methanol on Pd/Au Bimetallic Nanoparticles
	Arik	Beck	CO <sub>2</sub> hydrogenation to Methanol over Cu-In nanoparticles on ZnO
Electrochemical CO <sub>2</sub> Reduction	John	Lin	Probing CO <sub>2</sub> Electroreduction with In Situ Attenuated Total Reflection IR Spectroscopy
	Yusaku	Nishimura	Electrochemical Reduction of CO <sub>2</sub> over Bimetallic Electrocatalysts
	Alan	Landers	Ionic Compounds for Carbon Dioxide Electroreduction
	Yongfei	Ji	Transition metal dichalcogenides for CO <sub>2</sub> reduction
	McKenzie	Hubert	Understanding Electrocatalyst Deactivation Mechanisms for the CO <sub>2</sub> Reduction Reaction
Fuel Cells, ORR	Melissa	Kreider	Development of Transition Metal Nitride Catalysts for the Oxygen Reduction Reaction
	Ziyun	Wang	Predicting the Stability of Perovskites for Oxygen Reduction Reaction
	Hadi	Abroshan	Transition Metal Nitrides for the Oxygen Reduction Reaction
	Zhenghang	Zhao	Catalytic Mechanism of the oxygen reduction reaction in Co-doped C <sub>3</sub> N <sub>4</sub>
	Raoul	Flores	Screening Bulk Binary Transition Metal Stability Under Oxidizing Conditions

Fundamentals, Methods	Kristof	De Wispelaere	Effect of anharmonicity on adsorption and reaction thermodynamics on solid surfaces
	Paul	Jennings	Utilizing machine learning to accelerate a genetic algorithm for discovery of catalysts
	Roy	Kim	Materials characterization using transmission electron microscopy
	Martin	Hansen	Thermal Dehydrogenation of Ethane and Screening by Gaussian Process
	Aidan	Klobuchar	Development of Efficient Transition State Search Methods for Use with Large Datasets
	Brenna	Gibbons	Operando XAS Studies of Copper Silver Nanoparticles for the ORR
	Max	Hoffmann	Activity Trend Studies from Lattice Kinetic Monte Carlo
	Kristopher	Brown	Structural Changes in Catalytic Surfaces Induced by Applied Potentials
	Tom	Ludwig	Water structure on stepped copper surfaces
	Manuel	Kolb	Ultrafast chemistry to guide reactions on well-defined surfaces
Philomena	Schlexer	Size-dependence of the melting temperature of Au nanoparticles - A combined HR-TEM and molecular dynamics study	
Nitrogen	Arthur	Shih	Nature of SO <sub>2</sub> poisoned Cu-SSZ-13 Catalysts under Ammonia Selective Catalytic Reduction (NH <sub>3</sub> -SCR) Conditions
	Joshua	McEnaney	Ammonia Synthesis from N <sub>2</sub> and H <sub>2</sub> O at Atmospheric Pressure using an Electrochemical Cycling Strategy
	Aayush	Singh	Improving Selectivity for Electrochemical Ammonia Synthesis by Reducing the Rate of Proton-Electron Transfer
Water Splitting, Hydrogen Evolution	Andrew	Doyle	Exploring Geometric Effects in Oxygen Electrocatalysis
	Micha	Ben-Naim	Developing SrIrO <sub>3</sub> as an OER Catalyst for PEC Water-Splitting Devices
	Ieva	Narkeviciute	Si-Ta <sub>3</sub> N <sub>5</sub> photoanodes for solar water splitting
	Michaela	Stevens	Fundamentals and Industrial Applications: Understanding First Row Transition Metal (Oxy)Hydroxides as Oxygen Evolution Reaction Catalysts