

## AFOSR Molecular Dynamics and Theoretical Chemistry – Active Grants 2012

Principal Investigator	Institution	Grant Title	Link
Aikens, Christine	KANSAS STATE UNIVERSITY	STRUCTURE AND OPTICAL PROPERTIES OF NOBLE METAL NANOPARTICLES	
Anderson, Scott	UNIVERSITY OF UTAH	(MURI 08) - NANOCATALYSTS IN PROPULSION: MECHANISMS AND OPTIMIZATION	
Bartlett, Rodney	UNIVERSITY OF FLORIDA	MOLECULES AND THEIR INTERACTIONS	
Bergman, Robert	UNIVERSITY OF CALIFORNIA, BERKELEY	(NII) NOVEL CATALYTIC, SYNTHESIS METHODS FOR MAIN GROUP	
Bernskoetter, Wesley	BROWN UNIVERSITY	(YIP 11) Acrylate Formation from CO <sub>2</sub> and Ethylene by Catalysis	
Bernstein, Elliot	COLORADO STATE UNIVERSITY	STUDY OF HETEROGENEOUS CATALYTIC REACTIONS THROUGH GAS PHASE, NEUTRAL TRANSITION	
Betley, Theodore	HARVARD COLLEGE	(YIP 11) Bifunctional catalysts for CO <sub>2</sub> reduction	
Bocarsly, Andrew	PRINCETON UNIVERSITY	PHOTOELECTROCHEMICAL CONVERSION OF CARBON DIOXIDE TO ALCOHOLS: FORMATION CARBON-BASED FUELS VIA CARBON-CARBON BOND FORMATION	
Bowen, Kit	JOHNS HOPKINS UNIVERSITY	TOWARD THE DEVELOPMENT OF ALUMINUM CLUSTER-CONTAINING MATERIALS	
Bowers, Michael	UNIVERSITY OF CALIFORNIA SANTA BARBARA	LITIGATED METAL CLUSTERS - STRUCTURES, ENERGY AND REACTIVITY	
Brown, Seth	UNIVERSITY OF NOTRE DAME	(NII) Catalytic activation of nitrogen dioxide for selective synthesis	
Carter, Emily	PRINCETON UNIVERSITY	DESIGNING NEW MATERIALS FOR CONVERTING SOLAR ENERGY TO FUELS VIA QUANTUM MECHANICS	
Castleman, A. Welford	PENNSYLVANIA STATE UNIVERSITY	CLUSTER DYNAMICS: LAYING THE FOUNDATION FOR TAILORING THE DESIGN OF CLUSTER ASSEMBLED NANOSCALE MATERIALS	
Chirik, Paul	PRINCETON UNIVERSITY	(NII) - Synthesis of Fuels and Value-Added Nitrogen-Containing	
Christe, Karl	UNIVERSITY OF SOUTHERN CALIF	POLYNITROGEN CHEMISTRY	
Crim, Fleming	UNIVERSITY OF WISCONSIN	USING VIBRATIONS TO PROBE AND CONTROL PHOTOISOMERIZATION IN LIQUIDS	

Cuk, Tanja	UNIVERSITY OF CALIFORNIA BERKELEY	(YIP 12) In-Situ UV-VIS and IR Spectroscopy of Water Oxidation Catalysts	
Dlott, Dana	UNIVERSITY OF ILLINOIS CHAMPAIGN	ULTRAFAST DYNAMICS OF ENERGETIC MATERIALS	
Dukovic, Gordana	UNIVERSITY OF COLORADO	Photophysics and Photochemistry of Nanocrystals with Ultrashort Ligands	
Duncan, Michael	UNIVERSITY OF GEORGIA	Structure, Bonding and Surface Chemistry of Metal Oxide Nanoclusters	
Eichhorn, Bryan	UNIVERSITY OF MARYLAND	(NII) SYNTHESIS AND CHARACTERIZATION OF ALUMINUM BIMETALLIC NANOPARTICLES	
Engel, Gregory	UNIVERSITY OF CHICAGO	(PECASE) - HARNESSING SOLAR POWER NOVEL STRATEGIES FOR RATIONAL DESIGN OF PHOTOCATALYSTS AND PHOTOVOLTAIC MATERIALS	
Fayer, Michael	STANFORD UNIVERSITY	Dynamics and Interactions in Ionic Liquids and Surfaces	
Field, Robert	MASSACHUSETTS INSTITUTE OF TECHNOLOGY	AF-METASTABLE ELECTRONICALLY EXCITED ATOMS AND MOLECULES: EXCITATION TRANSFER IN SLOW COLLISIONS	
George, Steven	UNIVERSITY OF COLORADO	FABRICATION AND PROPERTIES OF ORGANIC-INORGANIC NANOLAMINATES USING MOLECULAR AND ATOMIC LAYER DEPOSITION TECHNIQUE	
Gordon, Mark	IOWA STATE UNIVERSITY	THEORETICAL STUDIES OF GROUP IVA AND GROUP IVB CHEMISTRY	
Halas, Naomi	RICE UNIVERSITY	PLEXITONICS: COUPLED PLASMON-EXCITON SYSTEMS WITH TAILORABLE PROPERTIES	
Heaven, Michael	EMORY UNIVERSITY	DIODE LASER PUMPED ALKALI VAPOR LASERS WITH EXCIPLEX-ASSISTED ABSORPTION	
Hernandez, Rigoberto	GEORGIA TECH	INCLUDING MOLECULAR STRUCTURE IN THE MULTI-SCALE MODELING OF NON-EQUILIBRIUM FLUID FLOWS	
Jin, Rongchao	CARNEGIE MELLON UNIVERSITY	ON THE EVOLUTION FROM NON-PLASMONIC METAL NANOCLUSTERS TO PLASMONIC NANOCRYSTALS	
Johnson, Mark	YALE UNIVERSITY	Optimizing catalysts for solar fuel production: Spectroscopic characterization of the key reaction intermediates	
Kaiser, Ralf	UNIVERSITY OF HAWAII	(HBCU 09) - UNTANGLING THE ENERGETICS AND DYNAMICS OF ELEMENTARY ATOMIC BORON REACTIONS	
Kanan, Matthew	STANFORD UNIVERSITY	(NII) - Local Electric Field Effects on Rhodium-Porphyrin and NHC-Gold Catalysts	
Khanna, Shiv	VIRGINIA COMMONWEALTH UNIVERSITY	CLUSTER ASSEMBLED MATERIALS FOR NANOENERGETIC APPLICATIONS AND CATALYSIS	

Knappenberger, Kenneth	FLORIDA STATE UNIVERSITY	(YIP 10) - MAGNETOPLASMONIC NANOMATERIALS: A ROUTE TO PREDICTIVE PHOTOCATALYTIC, LIGHT-HARVESTING AND FERROFLUIDIC PROPERTIES	
Kubiak, Clifford	UNIVERSITY OF CALIFORNIA SAN DIEGO	(MURI 10) NOVEL CATALYTIC MECHANISMS FOR THE CHEMICAL REDUCTION OF CARBON DIOXIDE TO ENERGY-DENSE LIQUIDS	
Landman, Uzi	GEORGIA TECH	(MURI 08) - ATOMIC-SCALE PRINCIPLES OF COMBUSTION NANOCATALYSIS	
Leone, Stephen	UNIVERSITY OF CALIFORNIA BERKELEY	ULTRAFast HIGH HARMONIC, SOFT X-RAY LASER PROBING OF MOLECULAR DYNAMICS	
Lineberger, W. Carl	UNIVERSITY OF COLORADO	Thermochemistry and Dynamics of Reactive Species	
Maginn, Edward	UNIVERSITY OF NOTRE DAME	MOLECULAR SIMULATION OF IONIC LIQUIDS: PHYSICAL PROPERTIES, MELTING POINTS, AND DROPLET COLLISION DYNAMICS	
Metiu, Horia	UNIVERSITY OF CALIFORNIA SANTA BARBARA	CATALYSIS BY ATOMIC-SIZED CENTERS: METHANE ACTIVATION FOR PARTIAL OXIDATION AND COMBUSTION	
Michl, Josef	UNIVERSITY OF COLORADO	EXTREMES IN OXIDIZING POWER, ACIDITY, AND BASICITY	
Miller, Thomas	CALIFORNIA INSTITUTE OF TECHNOLOGY	(NII) Exactly Embedded Wavefunction Methods for Characterizing Nitrogen	
Morokuma, Keiji	EMORY UNIVERSITY	THEORETICAL STUDIES OF GAS PHASE ELEMENTARY AND CARBON NANOSTRUCTURE GROWTH REACTIONS	
Nathanson, Gilbert	UNIVERSITY OF WISCONSIN	MOLECULAR BEAM STUDIES OF VOLATILE LIQUIDS AND FUEL SURROGATES USING LIQUID MICROJETS	
Nesbitt, David	UNIVERSITY OF COLORADO	STATE-RESOLVED THERMAL/HYPERTHERMAL COLLISIONAL DYNAMICS OF ATMOSPHERIC SPECIES	
Neumark, Daniel	UNIVERSITY OF CALIFORNIA BERKELEY	New Insights into Catalytic Sites: Spectroscopy of Metal Oxide Clusters	
Pfefferle, Lisa	YALE UNIVERSITY	(MURI 08) - NANOCATALYSTS FOR PROPULSION APPLICATIONS	
Rappe, Andrew	UNIVERSITY OF PENNSYLVANIA	CHEMICAL CONTROL OF EPITAXIAL OXIDE NANOSHELLS AND THEIR ROLE IN WATER SPLITTING	
Rioux, Robert	PENNSYLVANIA STATE UNIVERSITY	Dynamic Chemical and Structural Changes of Heterogeneous Catalysts	

Rogers, Robin	UNIVERSITY OF ALABAMA	DEVELOPING IONIC LIQUID KNOW-HOW FOR THE DESIGN OF MODULAR FUNCTIONALITY, VERSATILE PLATFORMS, AND NEW SYNTHETIC METHODOLOGIES FOR ENERGETIC MATERIALS	
Schatz, George	NORTHWESTERN UNIVERSITY	THEORETICAL STUDIES OF GAS-SURFACE AND GAS-PHASE DYNAMICAL PROCESSES	
Sen, Ayusman	PENNSYLVANIA STATE UNIVERSITY	SELF-MOVING CATALYTIC NANOMOTORS	
Sibener, Steven	UNIVERSITY OF CHICAGO	PRECISION GAS-SURFACE SCATTERING AND IMAGING STUDIES OF COMPLEX INTERFACES	
Subotnik, Joseph	UNIVERSITY OF PENNSYLVANIA	(YIP 11) Nonadiabatic Molecular Dynamics For Electron and Energy Transfer	
Troya, Diego	VIRGINIA TECH	ADVANCING THEORETICAL METHODS TO INVESTIGATE REACTIONS ON ORGANIC SURFACES IN VARIOUS ENERGY REGIMES	
Truhlar, Donald	UNIVERSITY OF MINNESOTA	ORBITAL-DEPENDENT DENSITY FUNCTIONALS FOR CHEMICAL CATALYSIS	
Voth, Gregory	UNIVERSITY OF CHICAGO	UNDERSTANDING THE DRIVING FORCES IN CATALYSIS	
Weiss, Emily	NORTHWESTERN UNIVERSITY	(YIP 10) - ELECTROCHEMICAL REDUCTION OF CO <sub>2</sub> AT A TiO <sub>2</sub> ELECTRODE USING QUANTUM DOTS AS MULTI-ELECTRON FUNNELS	
Willems, Katherine	UNIVERSITY OF TEXAS AT AUSTIN	(YIP-09) MAPPING LOCAL SHAPE-DEPENDENT ELECTROMAGNETIC FIELD ENHANCEMENTS IN SINGLE METALLIC NANOPARTICLES USING STOCHASTIC OPTICAL RECONSTRUCTION MICROSCOPY (STORM)	
Yarkony, David	JOHNS HOPKINS UNIVERSITY	FROM IGNITION TO PHOTOELECTRON SPECTROSCOPY CONICAL INTERSECTIONS IMPACT THE STUDY OF ENERGETIC MATERIALS	
Zanni, Martin	UNIVERSITY OF WISCONSIN	Dynamics of Photoexcitation at Nanostructured Carbon Interfaces	
Zare, Richard	STANFORD	KINETIC STUDIES OF REACTIONS IN SOLUTION USING FAST MASS SPECTROMETRY	
Zewail, Ahmed	CALIFORNIA INSTITUTE OF TECHNOLOGY	IMAGING UNDER EXTREME CONDITIONS	
Zheng, Junrong	RICE UNIVERSITY	(YIP 11) Chemical Dynamics at Surfaces of Metal Nanomaterials	