IN SEARCH OF A BRIGHTER FUTURE

2013-2014 ACTIVITY REPORT

KUTEM

KOÇ UNIVERSITY
TÜPRAŞ ENERGY CENTER

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KUTEM: THE FIRST ENERGY CENTER FUNDED BY A PRIVATE ENERGY COMPANY IN TURKEY TO CONDUCT RESEARCH ON NEW ENERGY TECHNOLOGIES

A SUSTAINABLE ENVIRONMENT

FOR JOINT INDUSTRY UNIVERSITY RESEARCH PROJECTS

ABOUT KUTEM

AN ENERGY RESEARCH CENTER AT KOÇ UNIVERSITY ESTABLISHED IN 2012 BY FUNDS FROM TÜPRAŞ, KUTEM'S GOALS ARE TO PROVIDE A SUSTAINABLE ENVIRONMENT FOR JOINT INDUSTRY UNIVERSITY RESEARCH PROJECTS, TO TRAIN STUDENTS FOR JOBS IN R&D IN INDUSTRY AND TO COMBINE FUNDAMENTAL AND APPLIED RESEARCH FOR INCREASING THE COMPETITIVE POWER OF TURKISH INDUSTRY.

EUR 3.3 m

Funds received from Tüpraş to strengthen research infrastructure

30

Faculty members in Engineering, Sciences and Administrative Science & Economics

FUELS

Concentrating on research activities mainly in fossil fuels, biofuels, solar fuels

KUTEM (Koç University Tüpraş Energy Center) is an energy research center at Koç University established in 2012 by a generous donation from Tüpraş. KUTEM, which functions as an umbrella for energy related research activities at Koç University, is the first energy research center funded by a private energy company in Turkey. The center consists of more than 30 faculty members in Engineering, Sciences and Administrative Science & Economics. Its goals are to provide a sustainable environment for joint industry university research projects, to train students for jobs in R&D in industry and to combine fundamental and applied research for increasing the competitive power of Turkish industry. The activities of the center are dictated by the Executive Council consisting of representatives from Koç University and Tüpraş.

KUTEM PROVIDES AN EASY ACCESS TO AN ENERGY RESEARCH FACILITY AT KOÇ UNIVERSITY AND BRINGS SCIENTISTS, STUDENTS, COMPANIES AND GOVERNMENTS TOGETHER TO TACKLE THE ENERGY CHALLENGE.

The research efforts at KUTEM are concentrated mainly in the area of fuels and divided into fossil fuels, biofuels and solar fuels. In the fossil fuels area, projects focus on improvement of the efficiency of fuel production technologies in industrial plants such as refineries and on development of novel catalyst systems for a wide variety of industrially important reactions. Development of new adsorbents for applications such as emission control, energy storage and separation processes for fuel processing is another focus area in this field. In the biofuels area, efforts are concentrated on using biomass feedstocks such as microalgae that do not compete with food. Significant research efforts are on developing new algae strains with high lipid content and growth rate by genetic modification and development of new photobioreactors for efficient growth of algae and development of new technologies for extraction of fuel from algae. In the solar fuels area, novel photocatalytic systems and devices are being developed for obtaining hydrogen by splitting water using sunlight. Even though the primary focus of the center is on fuels, the center provides support for many projects in the energy field such as lithium ion batteries, solar cells and thermal insulation.

KUTEM has 355 m^2 of laboratory space in the College of Sciences at Koç University and is equipped with laboratory instruments which are worth about 2 million €. The laboratory was designed to meet the critical research needs in the fuels area with state-of-the-art instruments and provides high-tech research opportunities for faculty members, researchers and students. Some of the equipment in the center are multiphase reactor systems, various spectroscopic devices for investigation of phenomena on surfaces, photobioreactors, various deposition units and high pressure volumetric adsorption units. KUTEM is intended to be an internationally recognized institution in the field of energy research, and thus contribute to Koç University's efforts in providing world-class education to its students.

KUTEM STRIVES TO EDUCATE NEW GENERATIONS WHILE PLACING A GREAT EMPHASIS ON SUSTAINABLE DEVELOPMENT. WHILE CENTER FACULTY HAVE BEEN EXTENSIVELY INVOLVED IN RESEARCH ACTIVITIES, THEY HAVE CONTINUED THEIR ACTIVE ROLE IN PROVIDING OPPORTUNITIES FOR EDUCATION, TRAINING, AND PROFESSIONAL DEVELOPMENT.

Other than Tüpraş, faculty at KUTEM also collaborates with both Turkish and multinational companies such as Aygaz, Aksa and BASF to develop new energy technologies. Moreover, the research projects are funded by international organizations as well as national funding agencies. For example, TÜBİTAK supports significant number of energy related projects at KUTEM. There are also research projects funded by the European Union 7th Framework program. The two European Union funded projects are on development of vacuum insulation panels for thermal insulation of buildings and porous coordination networks for CO_2 separations.

KUTEM also participates and promotes outreach activities in the energy field at Koç University. These include organization of seminars in the energy field by prominent researchers from around the world at Koç University, providing support for various energy related scientific conferences, supporting the activities of various student clubs at Koç University in energy related fields such as the Environmental Club and the Solar Powered Car Racing Club. KUTEM also gives seed funds to faculty at Koç University for innovative research projects in the energy field.

KUTEM strives to educate new generations while placing a great emphasis on sustainable development. The center is expected to attract bright young minds to the energy field and will also help to reverse the brain drain from Turkey by providing world class opportunities for young scientists. The center helps the faculty members to develop new energy related projects with seed funds, and therefore support new students with a grant of tuition and stipend. While center faculty is extensively involved in research activities, they have continued their active role in providing opportunities for education, training, and professional development.

KUTEM ALSO SEEKS TO DEVELOP NEW INTERNATIONAL PARTNERSHIPS THAT ARE BENEFICIAL AND CRUCIAL FOR THE NATION'S STRATEGIC ENERGY PLANS, WHILE ENHANCING AND DEEPENING RELATIONSHIPS WITH CURRENT PARTNERS. THERE ARE MANY ACTIVITIES INCLUDING BUT NOT LIMITED TO THE FOLLOWING:

- BECOME A CENTER WITH A REPUTATION IN GENERATION OF NEW IDEAS
- ESTABLISH NEW ACADEMIC COOPERATION FORMS WITH OUTSTANDING COLLEGES, UNIVERSITIES AND RESEARCH CENTERS FROM ALL AROUND THE WORLD.
- EXPLORE THE FUNDAMENTAL CONNECTIONS OF ENERGY TECHNOLOGIES TO ATOMIC, MOLECULAR, AND ELECTRONIC STRUCTURES.
- CREATE NEW KNOWLEDGE VIA THE RESEARCH OF ITS FACULTY AND APPLY THIS KNOWLEDGE FOR THE BENEFIT OF INDUSTRIAL PARTNERS.

WE OWE MUCH OF THIS SUCCESS TO OUR OUTSTANDING FACULTY, INTERDISCIPLINARY APPROACH, AND A PASSION FOR RESEARCH THAT DEFINES BOTH KUTEM AND KOÇ UNIVERSITY.

AS I LOOK AT THE WORK GENERATED BY KUTEM I SEE NOT ONLY AN INSPIRING RESEARCH COLLABORATION BETWEEN INDUSTRY AND HIGHER EDUCATION, I SEE WORLD CLASS OPPORTUNITIES AND A BRIGHT FUTURE FOR TALENTED YOUNG SCIENTISTS WORKING TOGETHER TO SOLVE THE ENERGY CHALLENGES THAT WILL SHAPE THE WORLD OF TOMORROW.

Our Energy Center KUTEM was founded by Koç University in collaboration with Tüpraş as a new and unique partnership to bring industry and higher education together to solve the energy problems of the world. Energy-related economic, security, and environmental threats continue to intensify national and global debates about energy leadership and competitiveness both in Turkey and the world, and the need to provide guidance for national strategic energy plans has never been greater.

In a short time KUTEM has established itself as an internationally recognized institution in the field of energy research, providing world-class education to students, and forming a strategic hub for international institutions, researchers and industry. We owe much of this success to our outstanding faculty, interdisciplinary approach, and a passion for research that defines both KUTEM and Koç University. As a university our mission is to conduct research that will make major contributions to humanity, sustainable life, and economy, in other words to create social impact and cultivate socially responsible generations.

KUTEM embodies and exemplifies this mission and the many industry-shaping technologies emerging from the center promise to transform how we generate and store fuel, helping to combat global warming, and reduce global reliance on fossil fuels.

Our researchers have already made great strides in improving the efficiency of fuel production technologies and developing new materials and techniques to safely store harmful chemicals and trap greenhouse emissions. In biofuels where costs and sustainability are critical, our research is lowering the cost of fuel extraction, and reducing the industry's reliance on biofuels sourced from edible food by developing technologies focused on microalgae as a biomass source.

As I look at the work generated by KUTEM I see not only an inspiring research collaboration between industry and higher education, I see world class opportunities and a bright future for talented young scientists working together to solve the energy challenges that will shape the world of tomorrow.

President Prof. Umran S. İnan

THIS RAPID GROWTH AND SYNERGY CREATED PROVES OUR CONFIDENCE IN KUTEM BEING A WORLD-RENOWNED RESEARCH CENTER IN THE ENERGY TECHNOLOGIES FIELD.

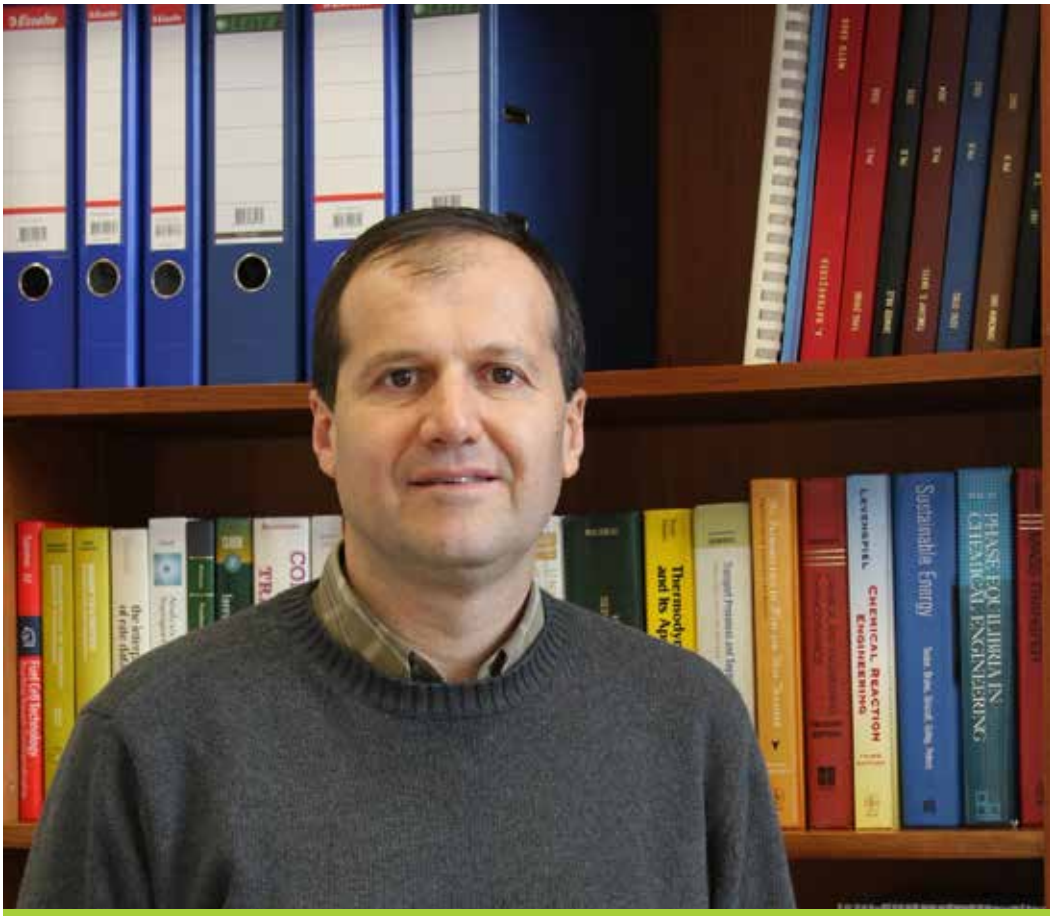
ENERGY HAS BECOME THE MOST IMPORTANT SUBJECT IN TURKEY AND ACROSS THE GLOBE. ENERGY ALSO CONSTITUTES A MAJOR PORTION OF A REFINERY'S EXPENDITURES. HENCE DEVELOPING TECHNOLOGIES FOR DEVELOPMENT AND USE OF ALTERNATIVE SOURCES, AND OPTIMIZING AND ENHANCING CURRENT TECHNOLOGIES ARE KEY FACTORS FOR TÜPRAŞ'S INNOVATIVE TECHNOLOGY SCOPE.

Tüpraş is fully aware that in order to maintain a competitive advantage and be successful in the global arena, it must reach a high level of technological competence. Thus, the Company carries out its R&D activities in line with its goal of becoming a globally competitive enterprise that leads the way in technological innovation. Tüpraş has planned its technological development and innovation processes and laid out its road maps, risk maps and technological action plans in order to carry out R&D activities successfully. In line with these plans, the Company aims to devise R&D projects that will contribute to both our country and the global energy industry. Including the investment in the R&D Center, Tüpraş's total R&D spending amounted to approximately TL 138 million. As part of its R&D efforts in 2014, Tüpraş successfully finalized a total of 10 projects approved by the Technology and Innovation Funding Programs Directorate (TEYDEB), and one project under the EU-funded 7th Framework Program. Currently, 13 projects approved by TEYDEB, one ARDEB 1003 project, and two EUREKA-labeled projects are still underway. In addition to the R&D projects funded by TÜBİTAK (The Scientific and Technological Research Council of Turkey) and the European Union, Tüpraş is currently carrying out 12 projects financed with its equity.

Energy has become the most important subject in Turkey and across the globe. Energy also constitutes a major portion of a refinery's expenditures. Hence developing technologies for development and use of alternative sources with optimizing and enhancing current technologies are key factors for Tüpraş's innovative technology scope. With that perspective Tüpraş established the Energy Systems Development Center - KUTEM in partnership with Koç University. Aiming to spearhead the development and use of alternative energy resources in our country under a university-industry partnership, KUTEM brings together industry and academia to carry out scientific research and innovation projects at international standards. KUTEM's primary fields of research include biofuel production, production of liquid fuel from recycled polymers, energy and fuel optimization, diagnostics of combustion mechanisms, laser ignition, hydrogen production and storage, transformation and utilization of solar energy, and emissions control. All of these studies are carried out under the umbrella of Tüpraş R&D Center.

It is our pleasure that KUTEM has 15 TÜBİTAK and 10 Tüpraş funded projects by 2014 with collaboration of several faculty of different research areas and several companies in energy field. This rapid growth and synergy proves our confidence in KUTEM's being a world-renowned research center in the energy technologies field.

Yavuz Erkut, Tüpraş General Manager



WE WILL STRIVE TO BECOME AN INTERNATIONALLY RECOGNIZED RESEARCH CENTER IN THE FIELD OF ENERGY.

I AM VERY HOPEFUL THAT THIS TREND WILL CONTINUE IN THE COMING YEARS NOT ONLY DUE TO THE GROWING IMPORTANCE OF ENERGY GLOBALLY AND BUT ALSO DUE TO TURKEY'S NEED TO DEVELOP NEW ENERGY SOURCES TO REDUCE ITS DEFICIT FROM CURRENT LEVELS.

I am very pleased about the completion of the first activity report of Koç University Tüpraş Energy Center (KUTEM). Over the past two years, we have put a lot of effort in setting up the research infrastructure of KUTEM. As a result, we now have an energy research facility at Koç University with state-of-the-art equipment, which we are all proud of. All of this would not have been possible without the generous donation from Tüpraş. Establishment of KUTEM has led to a significant increase in externally funded research projects in the energy field at Koç University. I am very hopeful that this trend will continue in the coming years not only due to the growing importance of energy globally and but also due to Turkey's need to develop new energy sources to reduce its deficit from current levels. This increase has also naturally led to an increasing number of M.S. and Ph.D. students at KUTEM who will be the leaders in the energy field in the future. I am especially excited about our joint research projects with Tüpraş and I am confident that Tüpraş will benefit from the outcome of these projects, thus helping us becoming a research center which can provide solutions to the problems of industry. I thank all the visionary people both in Tüpraş and Koç University administration that helped the establishment of this center. We will strive to become an internationally recognized research center in the field of energy.

Prof. Can Erkey
Koç University, Director of KUTEM

RESEARCH AREAS AND PROJECTS

BIOFUELS

WE BELIEVE THAT THE USE OF BIOFUELS WILL INCREASE IN THE COMING DECADE.

FOSSIL FUELS

IT WILL BE DIFFICULT TO MEET THE INCREASING ENERGY DEMAND FROM RENEWABLE ENERGY SOURCES IN THE NEAR FUTURE.

SOLAR FUELS

WE FOCUS ON MATERIALS FOR CONVERSION OF SOLAR TO CHEMICAL ENERGY.

Fossil Fuels

Our research efforts in the fossil fuels area concentrate on improving the efficiency of fuel production technologies, developing processes to reduce greenhouse emissions and helping enable the production of imported technologies in Turkey. We are also planning on working to develop technologies that will utilize the coal resources of our country for electricity and liquid fuel production. We hope that our center will thus be able to contribute to reduce Turkey's current account deficit.

Biofuels

We believe that the use of biofuels will increase in the coming decades and biofuels have potential as renewable fuels in Turkey. However, the biofuels which are in use today (ethanol, biodiesel) compete with edible food sources, lead to inflation of food prices, hunger and loss of forests. In order to prevent that, we carry out research to obtain fuels from sources which are not used for food such as algae, forest residues and switch grass. We are taking advantage of the strong biology and biotechnology research programs in our university.

Solar Fuels

As the fossil fuel reserves are expected to run out in approximately 100 years, it is necessary to find and develop alternative fuels. Promising ones are hydrogen which can be obtained by photocatalytic splitting of water and hydrocarbons by photocatalytic reactions of carbon dioxide and water vapor. Therefore, KUTEM concentrates on development of technologies for economical production of solar fuels and artificial photosynthesis.

FOSSIL FUELS

NOVEL TECHNOLOGIES

IN PROCESS CONTROL AND OPTIMIZATION, FUEL STORAGE AND ADSORPTIVE PROCESSES, CATALYSIS, REACTOR DESIGN AND DEVELOPMENT

OUR RESEARCH EFFORTS IN THE FOSSIL FUELS AREA CONCENTRATE ON IMPROVING THE EFFICIENCY OF FUEL PRODUCTION TECHNOLOGIES, DEVELOPMENT OF NOVEL NANOSTRUCTURED CATALYSTS, DEVELOPING NEW MATERIALS SUCH AS MEMBRANES AND ADSORBENTS FOR IMPROVING THE EFFICIENCY OF CURRENT SEPARATION TECHNIQUES AND NEW NANOSTRUCTURED SORBENTS TO TRAP GREEN HOUSE EMISSIONS.

Fossil fuels such as coal, petroleum and natural gas are expected to maintain their status as leading source of energy in the near future. For example, based on projections, they are expected to supply 80 percent of the energy needs in 2040. Moreover, between now and 2040, the consumption of natural gas and coal are expected to increase by 23.4% and 9.9%, respectively. Our research efforts in the fossil fuels area concentrate on improving the efficiency of fuel production technologies, development of novel nanostructured catalysts, developing new nanostructured materials such as membranes and adsorbents for improving the efficiency of current separation techniques and new nanostructured sorbents to trap greenhouse emissions.

In KUTEM, significant number of fossil fuel related projects are carried out by the faculty members. The research topics can be grouped under four categories which are Process Control and Optimization, Fuel Storage and Adsorptive Processes, Catalysis, Reactor Design and Development.

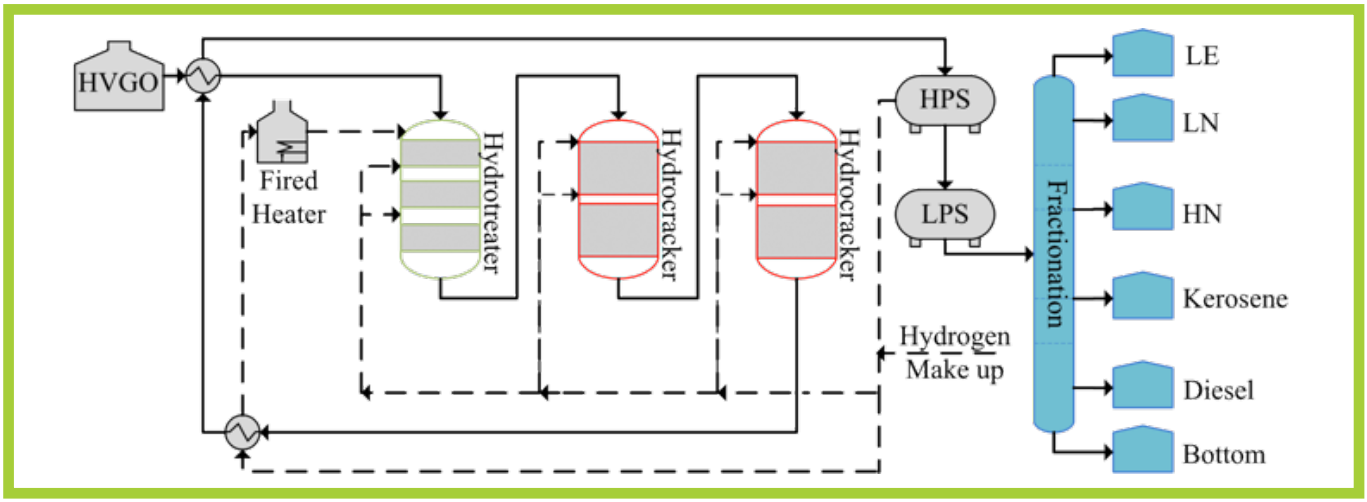
Process Control and Optimization

The general objective is to improve the operability, energy efficiency, product quality and profitability of industrial plants. This is accomplished through better modeling, real-time optimization and control. Especially for refineries with large throughputs and energy demands, the economic impact of performing advanced process control is very significant as small improvements lead to substantial economic savings. Prof. Yaman Arkun's research is implementing and improving state of the art modeling, control and optimization methods to industrial processes. Prof. Metin Türkay is developing models to capture interactions among economic and operational decisions at macro scale to incorporate demand and other environmental variations in the optimization of large-scale production complexes.

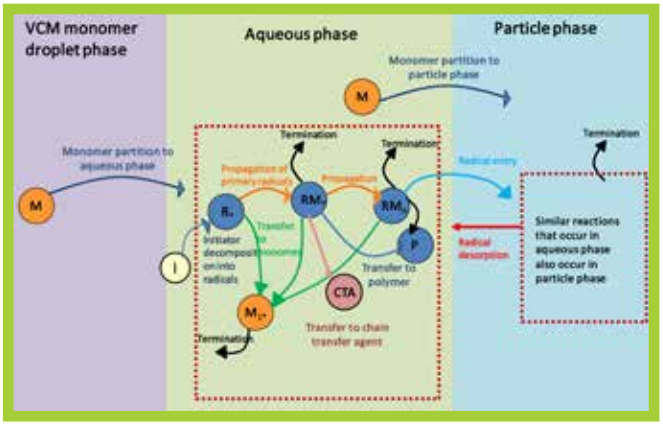
Real-time Optimization and Control of a Hydrocracker Unit

Prof. Yaman Arkun and his students developed a dynamic model for a hydrocracking plant at Tüpraş İzmit Refinery. The model is able to predict the real plant data under different operating conditions. A hierarchical plant-wide control system was also developed based on decentralized model predictive control. An improvement of 1 – 2% is expected in energy costs which accounts for 18% of total costs in the unit.

Flowsheet for a hydrocracker unit for converting heavy vacuum gas oil (HVGO)



Emulsion polymerization scheme

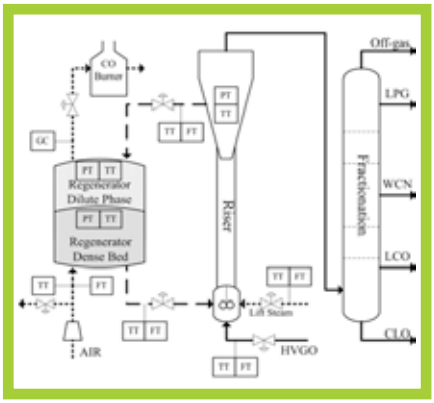


Modeling and Optimization of Entire Refinery

The complex interactions among different processes pose a significant problem for the optimization of refineries. Dr. Türkay is developing data-integrated approaches to modeling the complex interactions in a refinery through flow exchanges, shared utilities such as steam, water and electricity. In addition, the effect of variations in the demand for particular products and environmental variations are integrated into a holistic perspective of operations. The resulting model is solved by developing state-of-the-art discrete-continuous optimization algorithms to analyze the impact of decisions in refinery operations from economic and environmental perspectives. The results from this project are currently being applied to Tüpraş İzmit Refinery and the models for Aliağa and Kırıkkale refineries are being developed.

Industrial Application of Real Time Optimization and Control to Fluid Catalytic Cracking

Prof. Arkun and his students developed a dynamic model of a fluid catalytic cracking unit (FCC) at Tüpraş İzmir Refinery. The regenerator and the reactor were separately modeled from first principles. The model is validated against plant data. The dynamic model has been used for steady-state economic optimization and process control purposes. Using model predictive control and real time optimization algorithms, the plant can be operated at maximum profit subject to environmental and safety constraints. It is expected that energy costs will decrease when optimal operating conditions for different feeds are calculated and implemented in real-time.

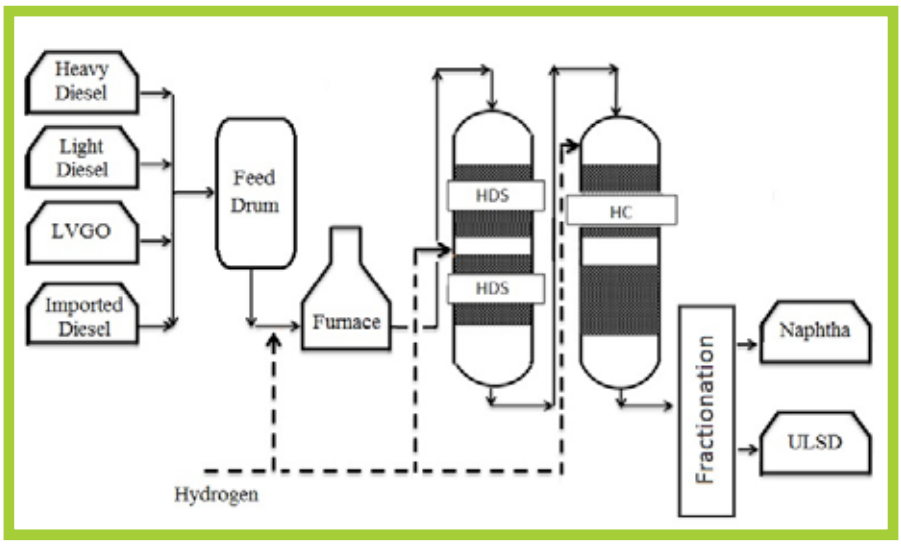


Flowsheet for a fluid catalytic cracking unit for converting heavy vacuum gas oil (HVGO)

Development of a Dynamic Model and Model Based Optimization and Control of a Semibatch Acrylonitrile-Vinyl Chloride Copolymerization Reactor

Dr. Kızılel, Prof. Arkun, and their students developed a dynamic mathematical model for a free radical emulsion copolymerization in a semibatch reactor for the production of acrylonitrile (AN) and vinyl chloride (VCM) copolymer. The approach used in this study is applicable to various comonomer systems, where average properties such as monomer conversion, copolymer composition, or polymerization rate for a typical emulsion copolymerization can be predicted. The particular model considers the changes in concentration of components in aqueous, particle and monomer droplet phases. The optimal AN/VCM feeding policy was determined using dynamic optimization which kept the AN to VCM ratio in the polymer close to one.

Flowsheet for a hydrodesulfurization unit



Modeling, Optimization and Control of an Industrial Diesel Hydroprocessing Plant

Prof. Arkun's research team modeled the diesel hydroprocessing plant at Tüpraş Kırıkkale refinery. The model is able to predict the sulfur consumption and diesel product properties closely.

The model was next used for the calculation of optimal steady-state operating point and the operational policy for the feed blending and the reactor units. The model's impact on improving profitability and reducing the sulfur content was found to be significant.

ADSORPTIVE TECHNOLOGIES

CAN ALSO BE USED FOR CHEMICAL ENERGY STORAGE SUCH AS STORAGE OF METHANE OR HYDROGEN FOR APPLICATIONS RANGING FROM AUTOMOTIVE TO STATIONARY POWER.

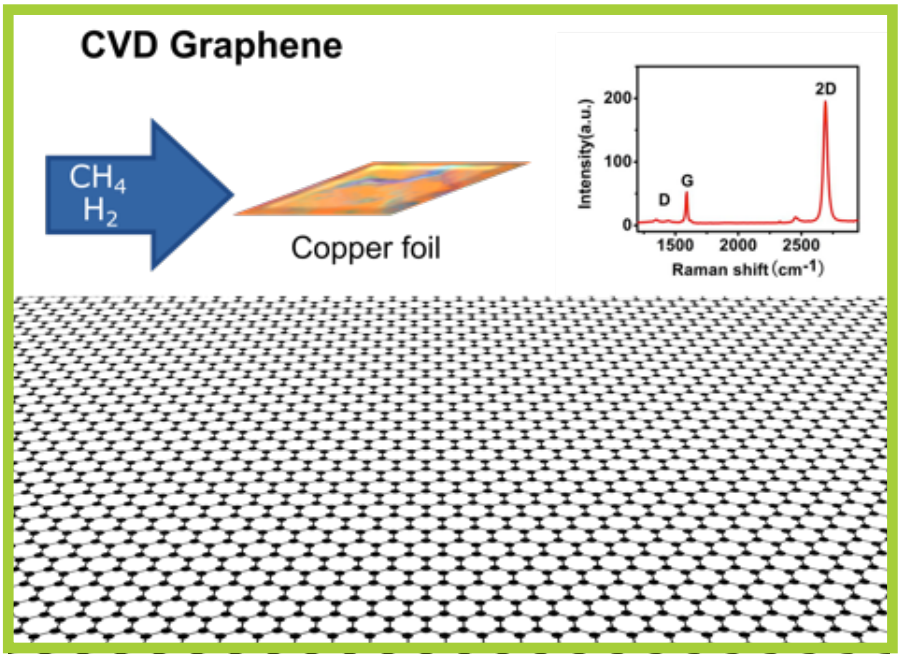
Fuel Storage and Adsorptive Processes

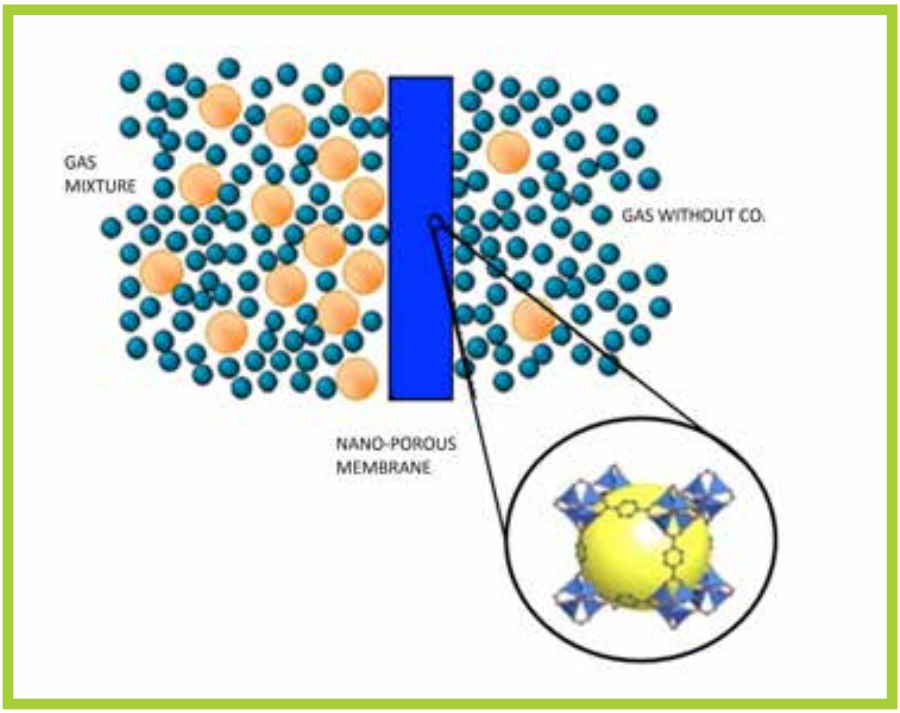
Adsorbents are used frequently in a wide variety of processes which are used in fuel production and energy storage. Adsorbents are generally nanostructured porous materials with large surface areas. Development of new efficient adsorbents is very important to reduce the costs associated with purification of gas and liquid mixtures in industrial plants, with removal of hazardous contaminants before emitting gases or liquid streams to the atmosphere and also for development of combined reaction/separation schemes such as catalytic distillation. Adsorptive technologies can also be used for chemical energy storage such as storage of methane or hydrogen for applications ranging from automotive to stationary power. Efforts at KUTEM are focused on development, synthesis and testing of new adsorbents and molecular simulation of adsorbents and modeling of adsorbent beds.

Graphene

Dr. Sarp Kaya and his students are investigating qualitatively and quantitatively hydrogen storage capability of graphene via formation of C-H bonds. Studies are carried out on atomically flat and corrugated graphene mono-, bi- and few layers. Hydrogenation-dehydrogenation mechanisms are investigated while probing the changes in electronic structure of graphene. Variations in C-C bond length due to corrugations, modifications in electronic structure due to metal substrate and the layer thickness are the key parameters of focus.

Spectroscopic investigation of formation of graphene on copper surfaces by chemical vapor deposition (CVD)





A membrane made from porous coordination network for gas separation

Computational Screening of Porous Coordination Networks as CO_2 Separation Membranes

There is a need to develop new materials exhibiting both high CO_2 selectivity and permeability in CO_2/CH_4 and CO_2/N_2 for large scale CO_2 separations to combat global warming. Dr. Keskin and her students are working on developing a new group of crystalline nanoporous materials named porous coordination networks (PCNs). The computational strategy being used is allowing them to rapidly choose the best PCN materials from a large group of candidates for making highly CO_2 selective membranes.

Aerogel Based Adsorbents

An aerogel is a special form of a highly porous material with a very low density which is composed of individual nano-sized particles that are connected to form a three dimensional network. Due to their large surface area, high porosities, and controllable structure, aerogels have high adsorption capacities for a variety of substances. Prof. Dr. Can Erkey and his students are developing novel composites of aerogels as adsorbents for methane storage, for CO_2 removal and also for humidity control.

AEROGELS AS ADSORBENTS

A PROJECT AT KUTEM FOCUSES ON DEVELOPING NOVEL COMPOSITES OF AEROGELS AS ADSORBENTS FOR METHANE STORAGE, FOR CO_2 REMOVAL AND ALSO FOR HUMIDITY CONTROL.

Development of Adsorbents for Methane Storage

Economic and environmental considerations have boosted interest in natural gas as a transportation fuel. A key challenge preventing the natural gas-driven energy future is the lack of effective, economic and safe on-board storage systems for CH_4, main component of natural gas. Design and development of new nanoporous materials that can store CH_4 efficiently and economically will be a crucial step towards a clean energy-driven future. In a joint project Dr. Alper Uzun, Dr. Seda Keskin and their students are using atomic level computations to develop novel hybrid materials containing metal organic frameworks (MOFs) to reach exceptionally high CH_4 storage performance under realistic operating conditions.

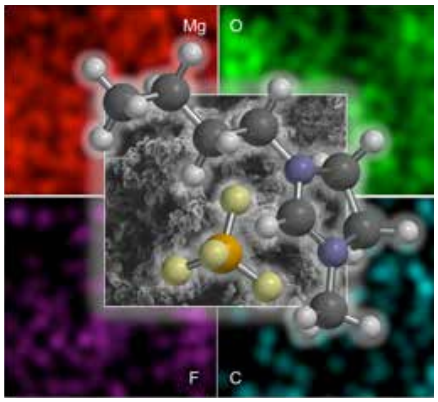
CATALYTIC SYSTEMS

EFFORTS AT KUTEM ARE DIRECTED AT DESIGNING AND DEVELOPING NOVEL CATALYTIC SYSTEMS, AT INVESTIGATING THE MECHANISMS OF REACTIONS BY COMPUTATIONAL AND SPECTROSCOPIC METHODS, AT CHARACTERIZATION OF CATALYSTS AND ELUCIDATING STRUCTURE ACTIVITY RELATIONSHIPS.

Catalysis

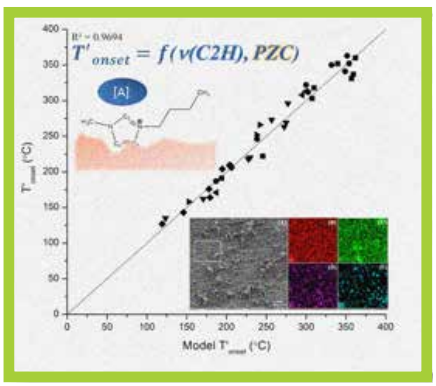
Catalysts which accelerate chemical reactions are essential components of processes for fuel production and storage. There is a demand to develop better catalysts to decrease current fuel production costs, to eliminate emissions of hazardous chemicals to our environment and also to make fuel extraction from unconventional energy sources economical. Efforts at KUTEM are directed at designing and developing novel catalytic systems, at investigating the mechanisms of reactions by computational and spectroscopic methods, at characterization of catalysts and elucidating structure activity relationships.

SEM/EDX image shows the uniform distribution of ionic liquid on metal-oxide surface.



Investigation of Structural Factors Determining the Applicability Limits and Performance of Imidazolium-Type Ionic Liquid Assisted Catalysts

Dr. Alper Uzun and his students are working on developing new catalysts by modifying conventional supported metal catalysts by a thin film of ionic liquid. The layer can impose a positive influence on the "chemical" properties of the catalysts by acting as a co-catalyst, either as an acidic function in a bifunctional catalyst or as a modifier or it may change the effective concentration of reaction intermediates and stabilize charged transition states or ligands to control the reaction pathways. However, it is not known exactly how these factors influence the catalytic performance. Approaches to solve this problem with IL-coated conventional supported metal catalysts on high-area supports are limited because of extremely complex nature of the active sites in such conventional supported metal catalysts. The novel approach here is to utilize the supported molecular metal catalysts to achieve an atomic-level understanding on how the IL coating layer interacts with the active sites and controls the reaction selectivity for the desired products. Supported molecular metal catalysts with IL layer are being prepared precisely to have well-defined and uniformly distributed active sites with controlled metal nuclearity on high area supports. This high degree of uniformity enables in-depth characterization of active sites and their interactions with IL layer before, during and after the reactions, ultimately enabling to achieve an atomic-level understanding on structure-performance relationships.



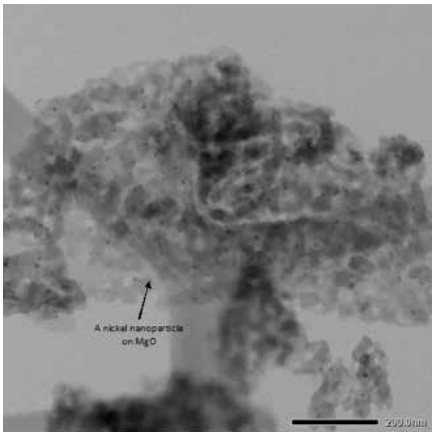
A simple model estimates the maximum tolerable temperatures of ionic liquids on metal-oxides as a function of (C2H) acidity of the imidazolium cation and the point of zero charge of the metal-oxide.

Preparation of Supported Single and Bimetallic Nanoparticle Catalysts by Supercritical Deposition

Bimetallic catalysts may have better activities and selectivities than their pure counterparts since the addition of another metal causes alterations in the electron density of the system and the changes of the metal-metal bond length that may lead to improved catalytic activity. The geometry has also important effects. For instance, one can improve the catalytic activity per amount of metal used by using a core-shell structure to provide the same catalytically active area in the shell with active and expensive metal (i.e. Pt) and with less active and cheaper metal in the core (i.e. Cu, Ni). Dr. Erkey and his students are developing novel carbon (carbon aerogel, graphene and their composites) supported nanoalloys for oxygen reduction reactions and also zeolite supported bimetallic catalysts for hydrocracking of heavy hydrocarbons into light and valuable products using supercritical deposition. They are investigating the effects of synthesis conditions on the properties and performance of the catalysts.

Development of Nickel-Based Catalysts as a Cheap Alternative to Ruthenium-Based Counterparts for the Production of Hydrogen from Ammonia

Dr. Uzun and his students are working to develop a cheap and highly efficient catalytic conversion technology for production of hydrogen from ammonia. Since no CO_2 is produced during its decomposition into hydrogen and nitrogen, ammonia offers clean and safe molecular level storage of hydrogen. Ruthenium-based catalysts are known as the best performing catalysts for this reaction, however, they could not be commercialized because of their high costs. Dr. Uzun and his students are focused on developing cheap nickel-based catalysts that are 100 times cheaper than their ruthenium counterparts. They are carefully examining the structure-performance relationships and tuning the structure of nickel-based catalysts based on this information to improve their catalytic performance to the levels comparable to that of ruthenium-based catalysts.



Well-dispersed nickel nanoparticles supported on MgO

Development of Alternative Fuel Additives and Determination of Their Fuel Competitiveness

This project carried out by Dr. Uzun and his students is on the development of a catalytic technology to produce fuel additives that can improve the fuel properties of either gasoline or diesel fuels. The focus is to tune the structure of solid acid catalysts and the operating conditions to optimize the catalytic performance and the product selectivity.

AT KUTEM, A TÜPRAŞ-FUNDED PROJECT THAT AIMS TO CONVERT LIGHT GASEOUS OLEFINS INTO LIGHT OR MID-RANGE DISTILLATES AS A SOURCE OF LIQUID FUELS IN PLUG FLOW REACTORS IS UNDER PROGRESS.

Reactor Design and Development

Reactors where chemical transformations take place are very important components of chemical processes used to produce fuels. Therefore, significant research efforts are exhausted in many laboratories around the world to develop new reactor systems with reduced capital and operating costs. Efforts at KUTEM are directed towards developing microchanneled reactors with high efficiencies, developing new reactors with increased selectivity to the desired products to reduce downstream separation costs and modeling complex reactor systems for fuel production.

Lab-on-a-chip

As a result of great advancement in material and fabrication technologies in recent years, devices have shrunk, and the strategy of "smaller is better" has begun to transform the world of fluidics as it has transformed the world of electronics. It is now possible to "print" miniature networks of channels with cross-sections typically on the order of tens of micrometers across – the width of a human hair. The ultimate goal is to create automated chemical laboratories and reactors called lab-on-a-chip that would fit on the palm of one's hand.

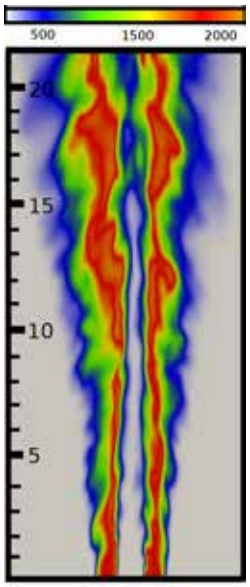
As the scale on which we study fluids decreases, the effects driving and dominating fluid motion change radically. At micron scales, fluids are primarily dominated by surface tension and viscous forces. The physics of microfluidic systems are well-described by continuum theory and flow is almost always laminar. Therefore computational fluid dynamics (CFD) can be used as a design tool and has a potential to replace most of the laboratory experiments. Prof. Muradoğlu and his students recently developed a finite-volume/front-tracking method for simulation of disperse multi phase flows in complex geometries and successfully applied to bubbles, drops and biological cells moving through microchannels, e.g., the motion, deformation and breakup of viscous drops in sinusoidally constricted capillaries, the mixing in droplet moving through a serpentine channel, mixing in a meandering channel that is segmented by gas bubbles, and formation of drops and bubbles by flow focusing in microchannels.

Development of a Technology to Produce Light and Mid-Distillates by Olefin Oligomerization

There is an increasing demand for diesel fuel and other light/mid-distillates. Converting light olefins into such hydrocarbons has a big potential of supplying this increasing demand as well as offering opportunities to improve the fuel properties of liquefied petroleum gas and light cracked naphtha. In this Tüpraş-funded project, Dr. Uzun and his students are aiming to convert these light gaseous olefins into light or mid-range distillates as a source of liquid fuels in plug flow reactors.

Turbulent Combustion

Prof. Muradoğlu and his students are working to advance modeling of turbulent flows involving complex chemical reactions and to develop efficient numerical techniques for the solution of turbulence and chemistry model equations with applications in real engineering design problems. Their current research focuses on the probability density function (PDF) modeling of turbulent reacting flows and the development of a consistent hybrid finite-volume (FV)/particle-based Monte Carlo method for solving the PDF model equations.



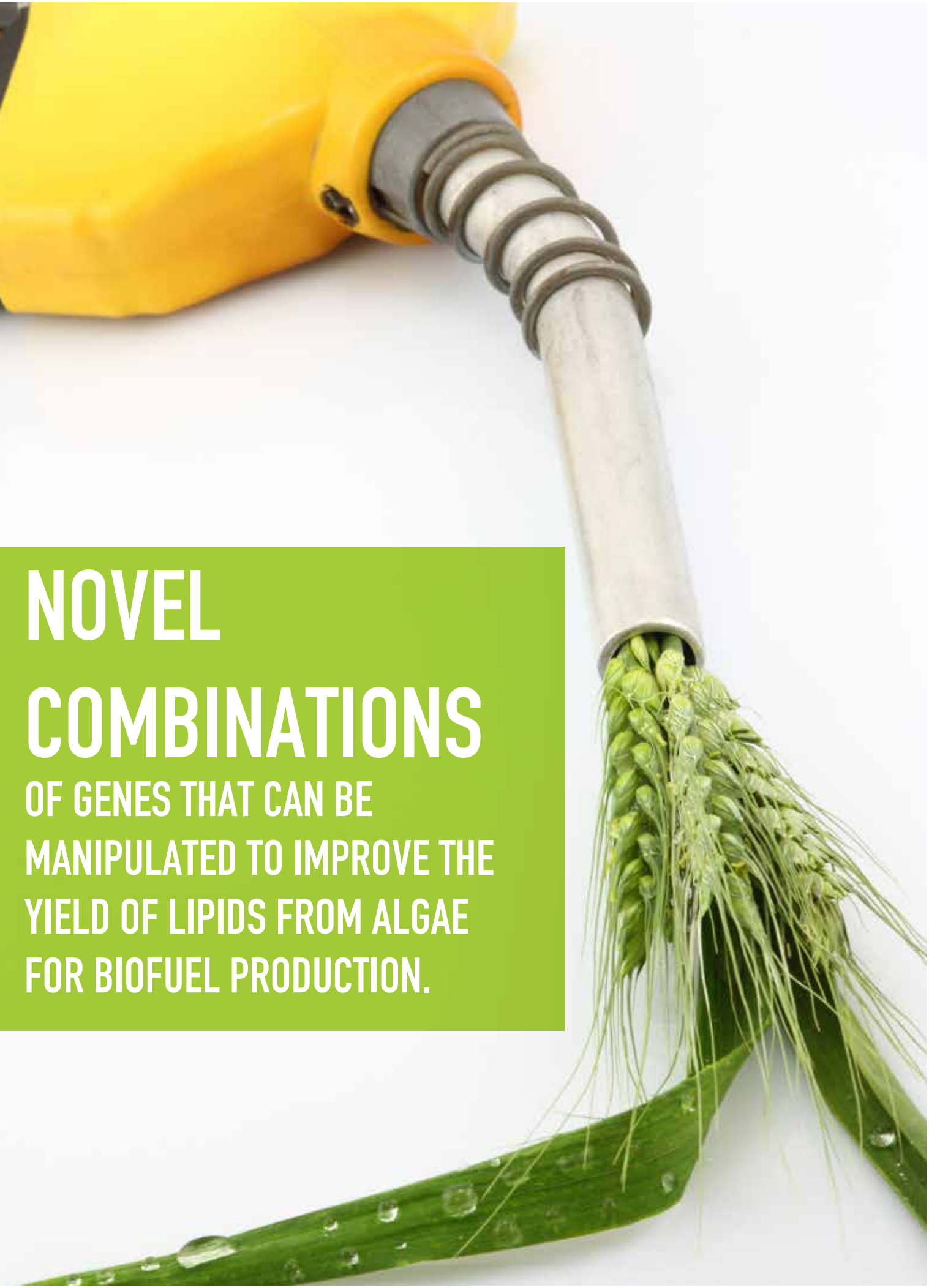
LES/PDF Simulation of Piloted Partially Premixed Methane/Air Diffusion Flame (Sandia Flame-D)

BIOFUELS

We believe that the use of biofuels will increase in the coming decades as more energy is obtained from renewable sources. The biofuels which are used today primarily for transportation (ethanol, biodiesel) are obtained from edible food sources, and therefore lead to inflation of food prices, hunger and loss of forests. In order to prevent such adverse effects, biofuels should be obtained from sources which are not used for food such as algae, forest residues and switch grass. Current research activities at KUTEM are concentrated on developing cost effective technologies for liquid fuel production using microalgae as the biomass source. To that end, efficient microbial strains are being screened, genetically modified and grown in photobioreactors.

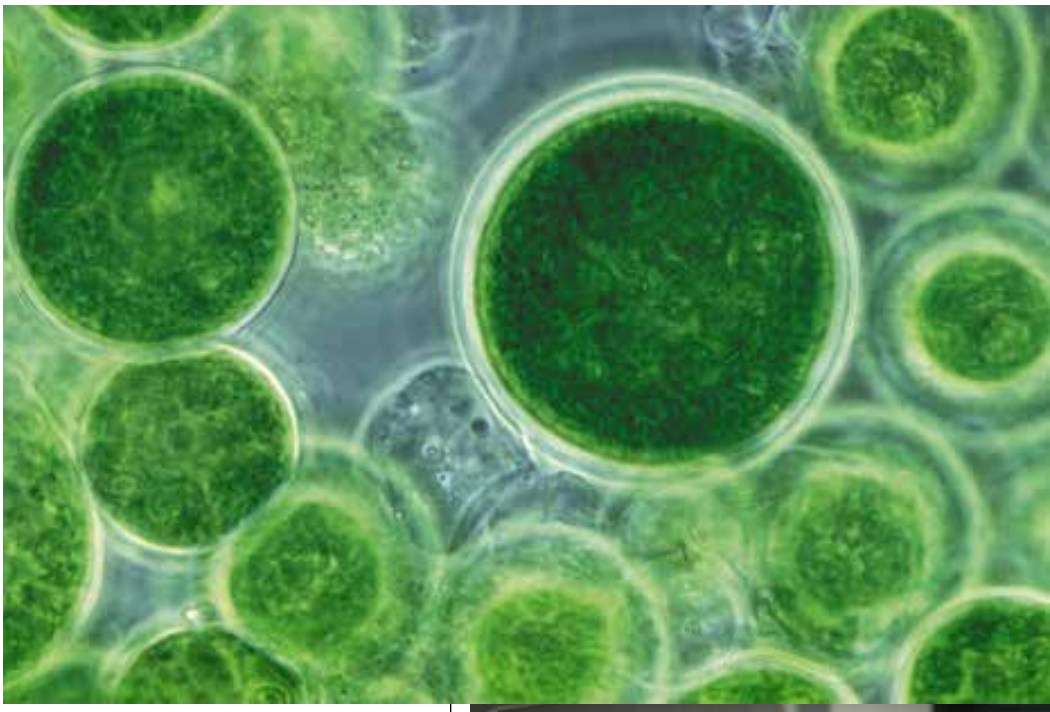
FOCUS

Research activities on biomass energy are concentrated on low cost and high efficiency conversion methods.



NOVEL COMBINATIONS

OF GENES THAT CAN BE MANIPULATED TO IMPROVE THE YIELD OF LIPIDS FROM ALGAE FOR BIOFUEL PRODUCTION.

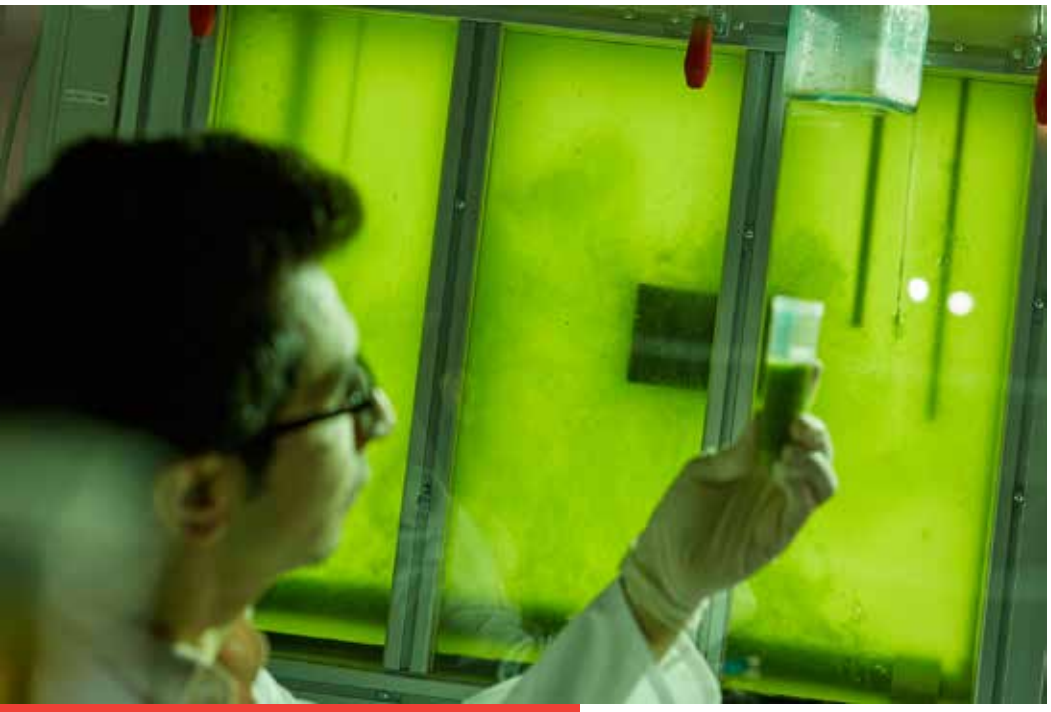


Strain Selection and Genetic Modification

Dr. Halil Kavaklı and his students are working on the generation of mutant *Chlorella vulgaris* strains which have high lipid content with high cell division rate using both chemical and physical (UV-light) mutagenesis. Their research already yielded a mutant, with a cell division rate 12% more than the wild type and which accumulates 50 % more lipid compared with wild type strain. They are currently using the RNA-Seq approach to decipher the effect of the mutations at genome wide level to identify affected pathway(s). They also started to build a pond race bio-reactor with a capacity of 10 000 Lt to grow *Chlorella vulgaris* at large scale and optimize growth conditions at large scale of both wild type and mutants to maximize lipid productivity.

Photobioreactor Development for Algae Growth

Mass cultivation of algae plays a critical role in CO_2 abatement. Photobioreactors allow a better control of the cultivation conditions than open systems. While higher biomass productivities are obtained with photobioreactors, contamination is also prevented.
The performance of the algal culture is dependent on an optimal design of a reactor and therefore, the reactor should provide optimum flow and gas exchange. Moreover, irradiance, concentrations of gas and nutrients are also critical in maximizing the yield of the process. Dr. Kızılel and his students are developing models which take into account these factors as well as gas-liquid mass transfer to predict oil yields in photobioreactors.

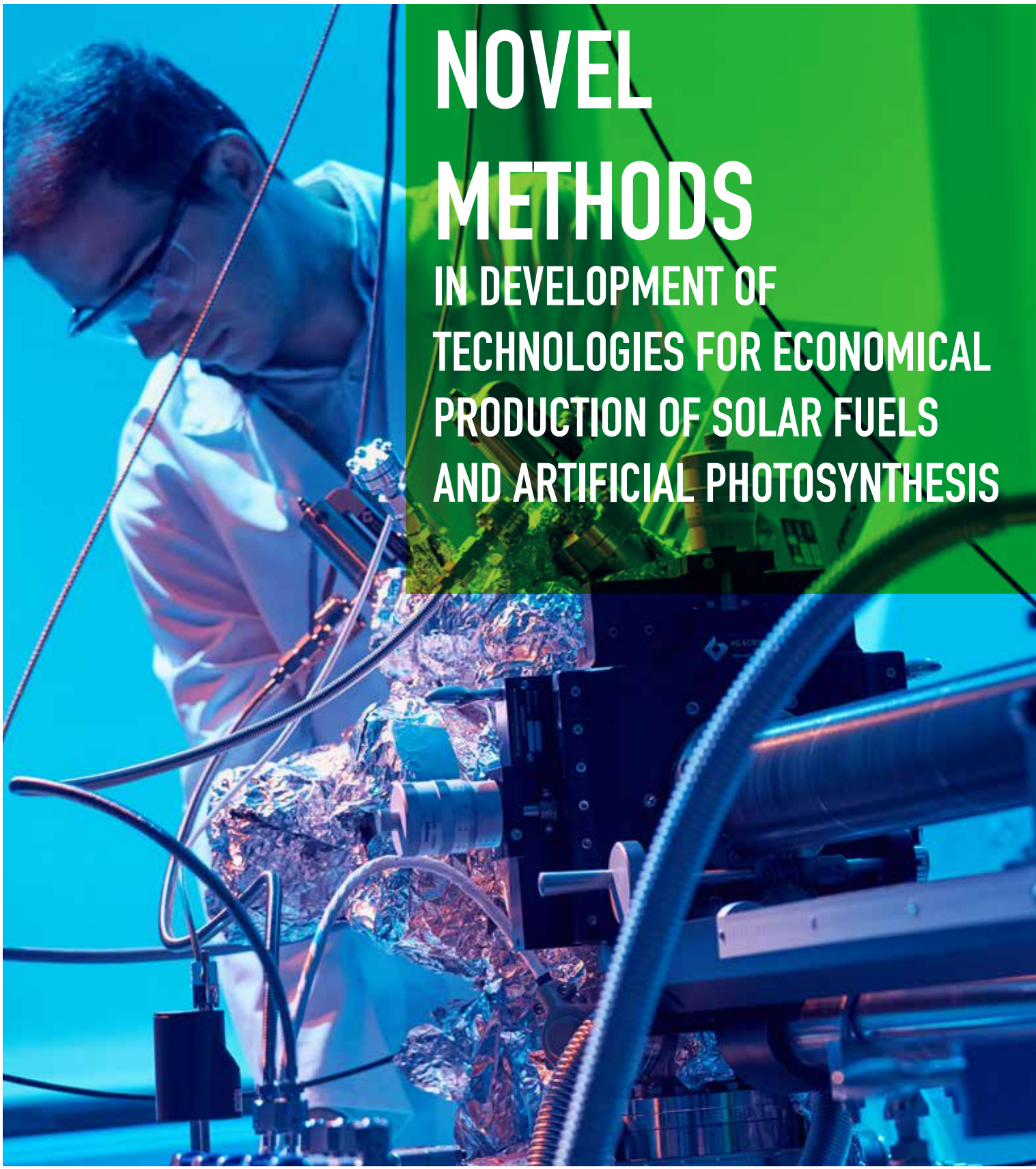


IT IS ANTICIPATED THAT DISCOVERY OF NEW TECHNOLOGIES WILL REDUCE THE PRODUCTION COST OF BIOFUELS FROM ALGAE SIGNIFICANTLY. OUR RESEARCH TARGETS THE REDUCTION OF PRODUCTION COST, MAXIMIZATION OF LIPID CONTENT AS WELL AS THE GROWTH RATE OF ALGAE.

Technologies for Harvesting and Fuel Production

A large fraction of the cost for production of fuels from algae is associated with harvesting the algae from photoreactors, extraction of the lipids from algae and conversion of the lipids to biodiesel by transesterification. It is anticipated that discovery of new technologies for these steps will make fuels from algae competitive on a price basis with other hydrocarbon based fuels. Prof. Can Erkey, Dr. Halil Kavaklı, Dr. Rıza Kızılel and their students are investigating supercritical extraction of algae oil from mutant strains of Chlorella vulgaris and trying to find the optimum conditions for maximum recovery of oil. They are also working on the application of a new technology called hydrothermal liquefaction which directly converts the algae slurry into a biocrude oil at high temperatures and pressures. The technology is particularly attractive since it eliminates the drying stage to recover the algae.

SOLAR FUELS



NOVEL METHODS

IN DEVELOPMENT OF TECHNOLOGIES FOR ECONOMICAL PRODUCTION OF SOLAR FUELS AND ARTIFICIAL PHOTOSYNTHESIS

PROMISING FUELS ARE HYDROGEN WHICH CAN BE OBTAINED BY PHOTOCATALYTIC SPLITTING OF WATER AND HYDROCARBONS BY REACTIONS OF CARBON DIOXIDE AND WATER VAPOR.

Solar energy can perhaps be used in the future to generate liquid or gaseous fuels which are termed solar fuels from abundant sources such as water and/or carbon dioxide. By developing systems which mimic photosynthesis, hydrogen fuel can be produced by splitting of water and hydrocarbon fuels such as methane or methanol by reactions of carbon dioxide and water vapor using photocatalysts. Once obtained in a renewable manner, such as via splitting water, hydrogen is one clean source of energy. From an application point of view, storing energy is as important as producing it, so there is urgent need to develop materials that have high storage capacities. Therefore, research efforts at KUTEM are concentrated on development of novel technologies for economical production of solar fuels.

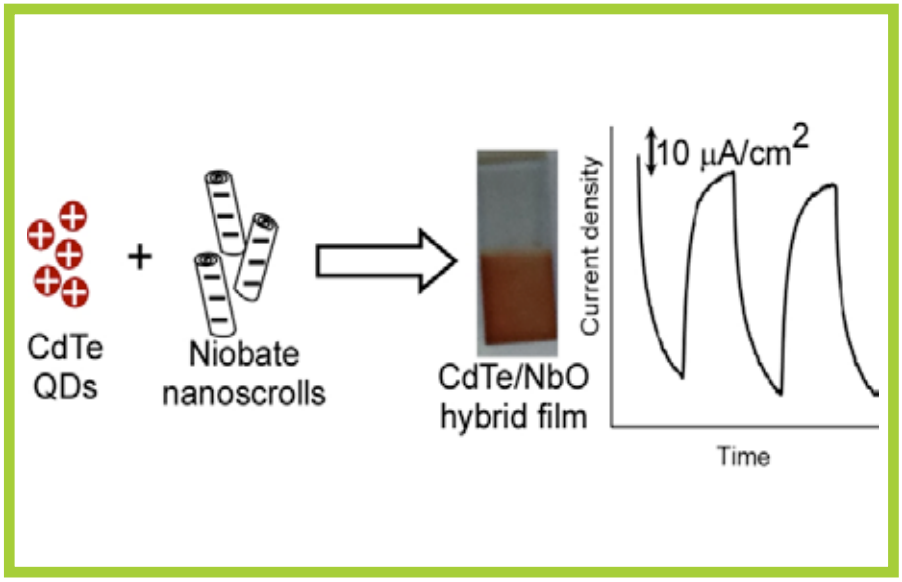
Photocatalyst Development

Electrochemical and photo-electrochemical reduction of CO_2 and CO to fuels (artificial photosynthesis) is one of the grand challenges in science and engineering. It has all the important ingredients: a very hard problem with the possibility of leading to game-changing technology, if successful. The main problem is the lack of suitable electro-catalysts – few materials work at all and all are extremely inefficient (high overpotentials).

High photocurrents produced by films of quantum dot sensitized layered niobate nanoscrolls

Development of Layered Materials

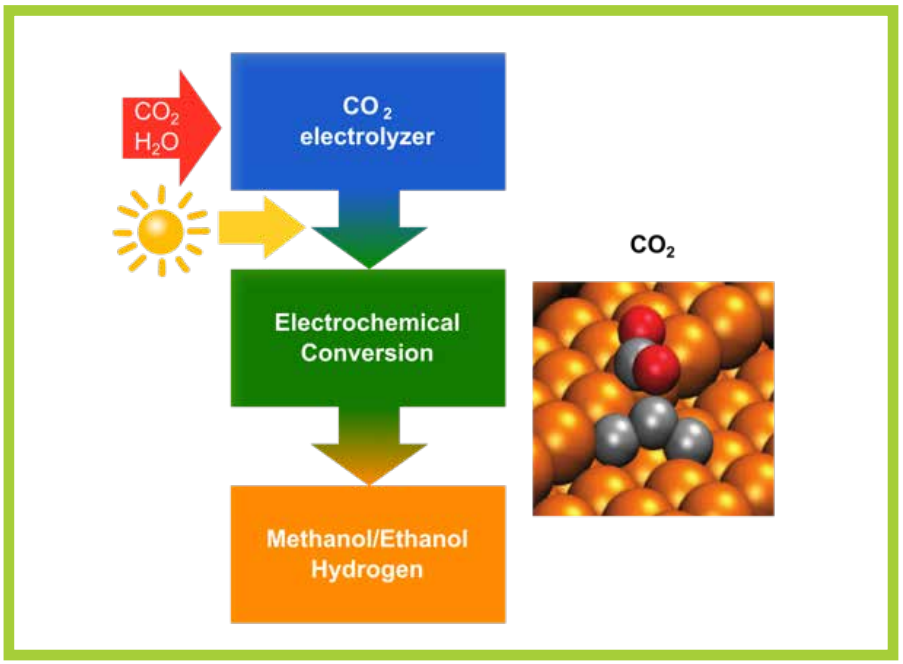
Dr. Ünal's group has been focused on the preparation, development and application of layered materials because of their very unique chemical and physical properties. These promising materials find applications in several fields such as ion-exchange, electrochemistry, photoelectrochemistry and photoluminescence. They have investigated the photoelectrochemical properties of quantum dot sensitized layered niobate nanoscrolls and found that their film produced 40 times higher photocurrent than reported values in the literature for similar systems. In addition, they have been studying electrochemical deposition of metal oxide and metal chalcogenides for energy applications. For example, $Cd_xZn_{1-x}S$ (CdZnS) has been found to be a promising material for buffer layers in copper indium gallium (di)selenide (CIGS) and CdTe solar cells. In their research, they explore photoelectrochemical properties of CdZnS films synthesized by electrochemical deposition. As-prepared films display significantly enhanced photocurrent compared to the literature. The promising current-voltage characteristics suggest possibility of efficient solar cell construction.



IN A KUTEM STUDY, PHOTOELECTROCHEMICAL PROPERTIES OF CDZNS FILMS SYNTHESIZED BY ELECTROCHEMICAL DEPOSITION ARE EXPLORED. THE FILMS DISPLAY SIGNIFICANTLY ENHANCED PHOTOCURRENT COMPARED TO THE LITERATURE.

Electrochemical CO_2 and CO Reduction to make Methanol Fuel

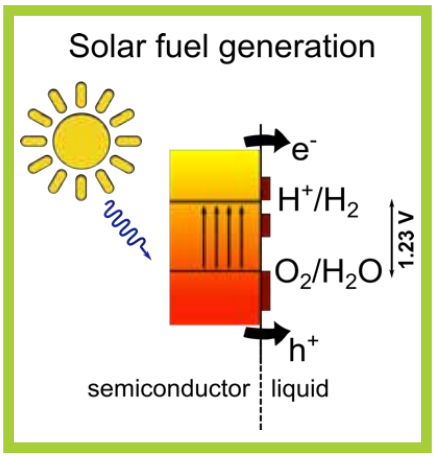
One of the best known catalysts is copper, but not much is known about the reasons behind this reactivity. The aim this project is to search for new catalytic materials for (photo)electrochemical CO_2 reduction using a rational material design strategy involving synthesis of potentially interesting copper alloys. Possible strategies for changing the surface properties to achieve lower overpotentials are being investigated by following trends in catalytic activity from one metal to the next. By this means the factors determining the product selectivity will be revealed.

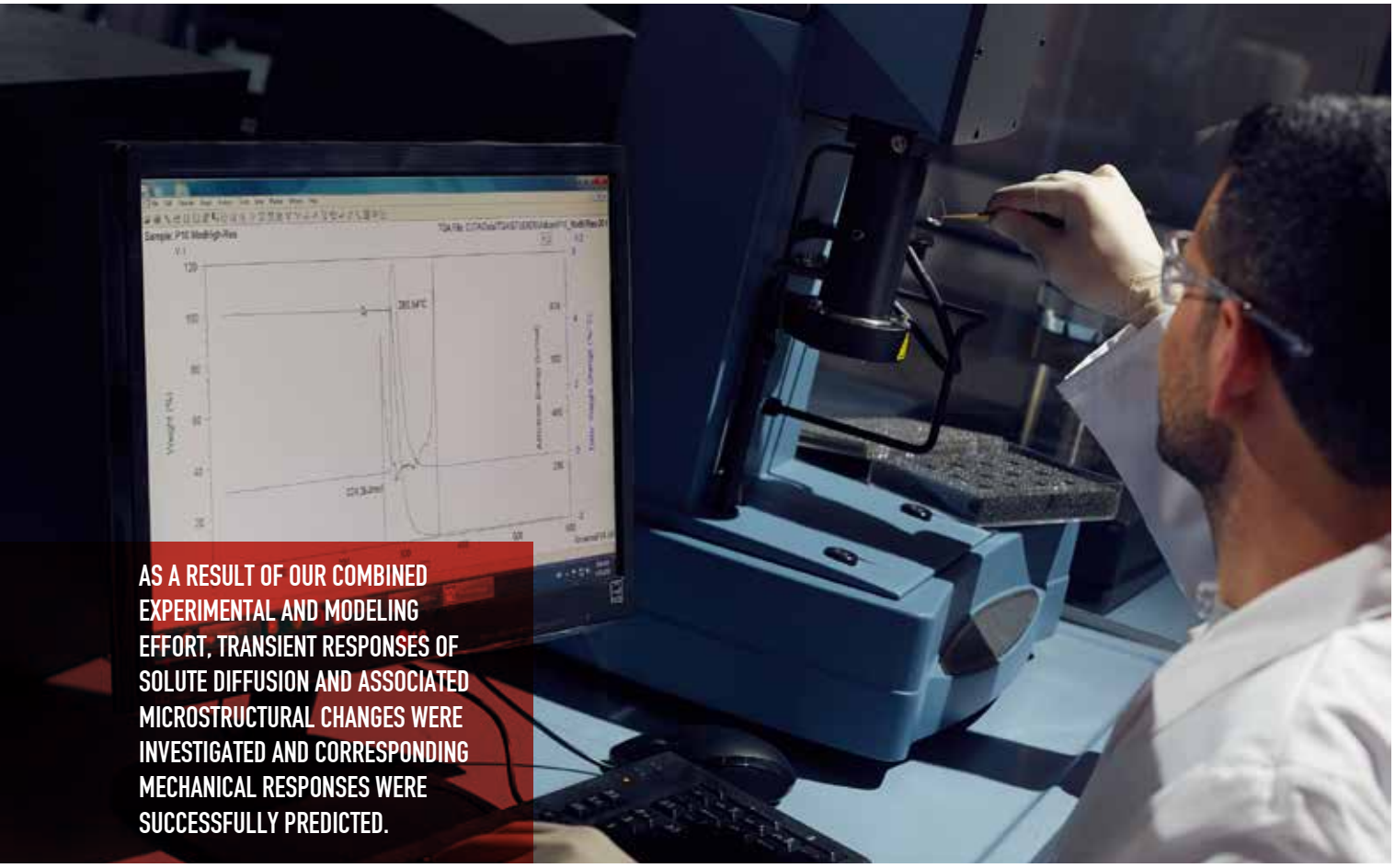


Scheme for generating alcohols and hydrogen from carbon dioxide and water using sunlight

Developing Highly Efficient and Stable Photo-anodes for Photo-electrochemical Cells

It is necessary to understand solid-solid and solid-liquid interfacial chemical processes at the atomic-molecular level and to use this knowledge to stimulate advances in photo-electrochemical energy conversion. Semiconductor liquid junctions offer the potential for hydrogen production by splitting water using light, but this technology is far from being widely accepted because of poor efficiency. Band positions of bismuth vanadates ($BiVO_4$) and tantalum oxynitrides (TaON) with respect to redox potentials of water splitting are appropriate and band gaps are rather suitable for absorbing a big portion of the solar spectrum. This implies that these materials have the potential to produce hydrogen and oxygen under visible light. However, electron-hole pair recombination losses, poor electrical conductivity, and interfacial losses are known to be main limiting factors. Dr. Sarp Kaya and his students are aiming to engineer the band structures of bulk and thin film $BiVO_4$, TaON, and TiO_2 as a passivation and hole blocking-hole mirror layer using doping, morphology control, surface modification, construction of composite structures in order to improve solar to hydrogen conversion efficiency.

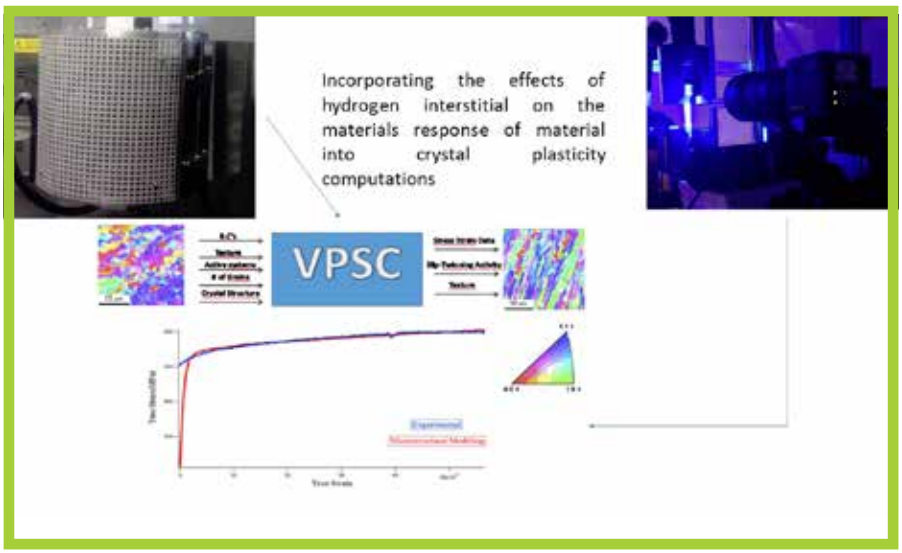




AS A RESULT OF OUR COMBINED EXPERIMENTAL AND MODELING EFFORT, TRANSIENT RESPONSES OF SOLUTE DIFFUSION AND ASSOCIATED MICROSTRUCTURAL CHANGES WERE INVESTIGATED AND CORRESPONDING MECHANICAL RESPONSES WERE SUCCESSFULLY PREDICTED.

Separation, Storage and Conversion of Solar Hydrogen

Solar hydrogen is generally produced from water as a mixture of hydrogen and oxygen. Therefore, technologies are needed to efficiently separate hydrogen from oxygen since current technologies are cost prohibitive. Moreover, hydrogen generally needs to be stored before using it as a fuel or converting it to electricity. Efforts at KUTEM are directed at developing new materials with high hydrogen adsorption capacities with favorable kinetics, understanding the interactions of hydrogen with various materials at the atomic scale both by experiments and simulations, development of novel membranes for separation of oxygen and hydrogen and developing cost effective fuel cells for converting hydrogen into electricity.



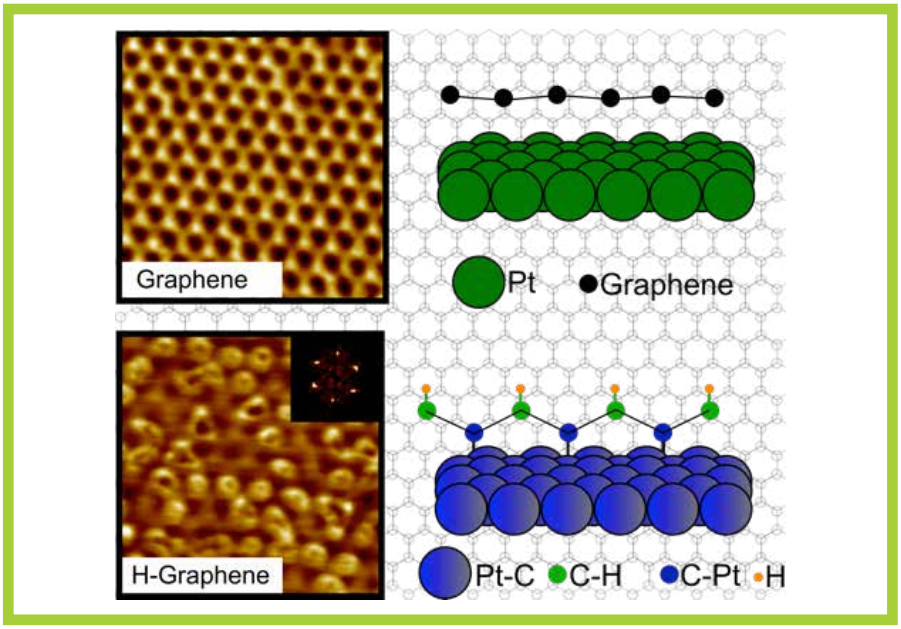
Tackling a Critical Problem in Hydrogen Storage Through a Multi-Scale Modeling Approach: Crack Propagation in the Presence Of Hydrogen Embrittlement

Dr. Demircan Canadinç and his students are investigating the storage of hydrogen in metal containers. The hydrogen effect on the mechanical behavior of iron was experimentally investigated at low strain rates. Based on experimental results, classical Voce hardening scheme was modified to account for the shear stresses imposed on arrested dislocations due to the surrounding hydrogen interstitials. This study presented a physically based crystal plasticity formulation, which was successfully applied to iron matrices. The modified visco-plastic self-consistent model successfully predicted the role of hydrogen interstitials on the macroscopic deformation response of iron polycrystal. As a result of combined experimental and modeling effort, transient responses of solute diffusion and associated microstructural changes were investigated and corresponding mechanical responses were successfully predicted. Despite the fact that the work focuses on iron-based matrix, the outcomes will be applicable to all metallic storage materials to be utilized in hydrogen-fueled applications.

Modifying Hydrogenation and Nitrogenation Capabilities of Graphene

Graphene as a two dimensional carbon material with high surface area has great potential but the nature of the chemical bond between hydrogen and carbon must be understood well. Dr. Sarp Kaya and his student are working on this side of the project.

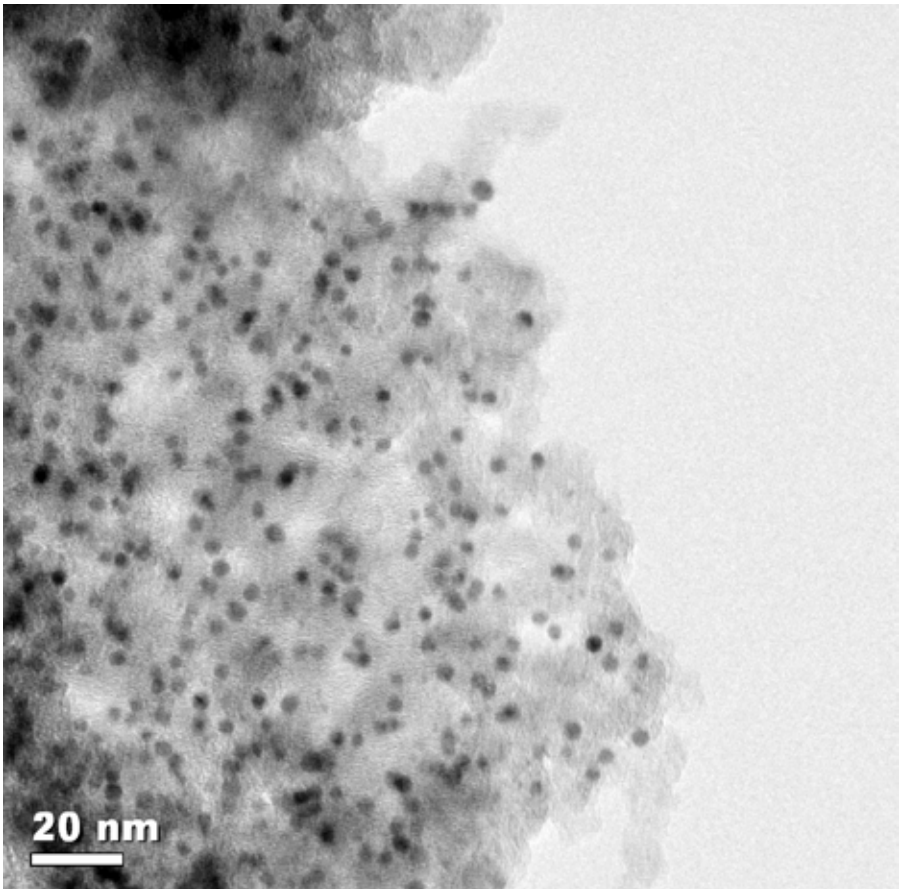
Energy in the chemical bond of hydrogen molecule can be converted into electricity using devices known as fuel cells where hydrogen and oxygen meet to form water. Platinum is used as a catalytically active electrode material to facilitate this reaction but cheaper alternatives are needed in order to have widespread use. Nitrogen doped graphene is a cheap alternative fuel cell cathode on which limiting oxygen reduction reaction takes place. The aim of the project is to understand the C-N bonding in functionalized graphene and develop means to improve its activity in such a way that nitrogenated graphene could be considered as viable material for fuel cell applications.



Modifying hydrogenation and nitrogenation capabilities of graphene

Hydrogen Fuel Cells

The activity of a Polymer Electrolyte Membrane Fuel Cell (PEMFC) is limited by the rate of the oxygen reduction reaction taking place on cell's cathode. Pt is the most active catalyst facilitating this reaction, but the problem is that Pt is scarce and thus is expensive preventing worldwide use of fuel cells. An alternative catalyst or modified Pt is required. Carbon aerogels (CA) are attractive materials as electrocatalyst supports for PEMFCs. The ideal support should have a high accessible surface area to improve the dispersion of platinum nanoparticles, suitable pore size and pore volume to enable efficient transport of ions, high electronic conductivity, and high stability. Prof. Dr. Can Erkey and his students are investigating the use of CAs as an electrocatalyst support. They investigated the effects of sol-gel parameters on the pore volume and average pore size of CAs. Decreasing resorcinol to water ratio was found decrease the density and increase the average pore size. It was possible to adjust the average pore size from 3 nm to 22 nm by changing the reactant concentrations in the sol-gel process. Platinum -copper nanoparticles were deposited on to CAs by the supercritical deposition method. The resulting nanoparticles were very well dispersed on the CA surface with average crystallite sizes around 3 nm. The electrochemical activity of the CA based electrocatalysts was investigated by cyclic voltammetry. The electrochemical surface areas were found to decrease with increasing crystallite size.



Transmission electron microscopy image showing carbon aerogel supported Pt-Cu nanoalloy particles (average particle diameter: 3.6 nm, composition: $Pt_{77}Cu_{23}$)

OTHER ENERGY RELATED RESEARCH ACTIVITIES

NOVEL APPROACHES

IN MORE EFFICIENT USE OF ENERGY RESOURCES AND IN DEVELOPMENT OF DELIBERATE POLICIES OF ENERGY SECURITY

Determination of Density and Viscosity of Fluids and Fluid Mixtures at High Pressures

Drs. Alaca, Kiraz and Erkey are developing a technique to measure density and viscosity of fluids and fluid mixtures at a wide range of pressures and temperatures by using frequency response measurements of microcantilevers. For that purpose, a new experimental setup was developed where a microchip containing ferromagnetic nickel microcantilevers and an electromagnetic coil are placed inside a high pressure sample chamber which can operate up to 150 ^{0}C and 413 atm. The procedure involves driving of microcantilevers with AC magnetic field at varying frequencies and detecting the laser deflections from the driven cantilevers with a quadrant photodiode (QPD). Subsequently, frequency response data were used to extract density and viscosity with a model that describes the oscillatory behavior of microcantilevers. These calculations can be significant in different application areas in the energy field. For example, density and viscosity of carbon dioxide or carbon dioxide mixtures can be used in studies related to lowering carbon dioxide emissions to the atmosphere.

Optimization of Energy Mix for Turkey

Turkey is going through fast industrial development and the energy demand is increasing proportional to this development. The meeting of energy demand using a combination of various fossil and renewable sources is required. Dr. Türkay is developing a dynamic model to incorporate changing energy demand profiles from different sectors such as industry, commerce, housing and services and also the available capacity with techno-economic developments for energy generation in Turkey. The dynamic model provides useful insights into the energy mix problem of Turkey for investment and energy policy decisions.

Development of Silver Chalcogenide Sensitized Solar Cells

Quantum dots (QDs) are exploited in a variety of energy related fields including solar cells, LEDs, sensors and lasers. Compared to organic dyes, QDs offer higher photobleaching threshold and narrow spectral bands, which make them excellent fluorescent tags with better sensitivity. Ability to excite various size QDs simultaneously with a single excitation wavelength provides an opportunity to create multicolor arrays. Silver chalcogenides are ideal alternatives materials for new generation solar cells due to their narrow band gaps, high electron conductivity and low toxicity. Dr. Uğur Ünal, Dr. Funda Yağcı Acar and their students are developing silver chalcogenides as sensitizers along with TiO_2 and ZnO hosts for solar panel applications. The efficiency of these materials for conversion of solar energy into electricity is also under investigation.

Nanostructured Composites of Silica Aerogels for Thermal Insulation

Improvement of current thermal insulation systems in buildings, appliances, manufacturing facilities and transportation are expected to lead to substantial reductions in energy expenditure. Aerogels are nano structured materials with intriguing potential to replace conventional insulation materials since they have significantly lower thermal conductivities due their very low density, highly porous structure and pore sizes that are on the order of nanometers. Prof. Can Erkey and his students are developing aerogel based thermal insulation systems for a wide variety of applications ranging from refrigerators to buildings. These include transparent vacuum insulation panels which uses aerogels as core materials and composites of aerogels with polymers for enhancement of mechanical strength of conventional aerogels. Different kinds of aerogels such as silica, resorcinol-formaldehyde, carbon and alginate aerogels are being synthesized. The effects of pore properties such as average pores size, pore volume and pore size distribution as well as the solid structure on thermal conductivity are being investigated both by simulations and experiments.

Analysis of Electromobility from a Sustainability Perspective

Electromobility has the potential to provide significant improvements on the energy efficiency of the transportation sector. The environmental impact from electromobility highly depends on the energy mix of a country for electricity generation. Dr. Metin Türkay and his students are developing discrete-continuous optimization models and multi-objective optimization algorithms for the analysis of electromobility from a sustainability perspective including economic and environmental impacts. The initial results indicate that a 10% conversion of existing vehicles to electromobility would result in 65% reduction in the cost of energy and 70% reduction in CO_2 emissions for these vehicles considering the electricity generation profile of Turkey.

ENERGY CONTENT OF

A CLASSICAL BATTERY SCALES LINEARLY WITH ITS MASS. WE HAVE RECENTLY PROVEN THAT A QUANTUM BATTERY CAN STORE ENERGY PROPORTIONAL TO THE SQUARE OF ITS MASS.

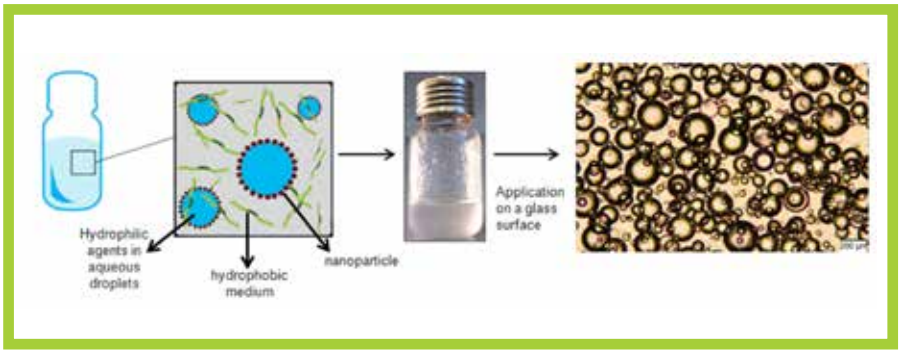
Elimination of Ice Formation on Functional Coatings

Polymer composites consisting of small hydrophilic pockets homogeneously dispersed in a hydrophobic polymer matrix are important in many applications where controlled release of the functional agent from the hydrophilic phase is needed. As an example, release of salt in anti-icing application can be mentioned.

Dr. Seda Kızılel and Prof. Levent Demirel and their students developed a method for preparation of such a composite material consisting of small KCOOH salt pockets distributed in a styrene-butadiene-styrene (SBS) polymer matrix and demonstrated its effectiveness in anti-icing coatings. The mixtures of the aqueous KCOOH and SBS-cyclohexane solutions were firstly stabilized by adding silica nanoparticles to the emulsions and, even more, by gelation of the aqueous phase by agarose. The emulsions were observed in optical microscope to check their stability with time and characterized by rheological measurements. The dry composite materials were obtained via casting the emulsions onto the glass substrates and evaporation of the organic solvent. Composite polymer films were characterized by water contact angle measurements. The release of KCOOH salt into water and the freezing delay experiments of water droplets on dry composite films demonstrated their anti-icing properties. It was concluded that hydrophobic and thermoplastic SBS polymer allows incorporation of the hydrophilic pockets/phases that opens the possibility for controlled delivering of anti-icing agents from the composite.

Coherence Capacitor, Quantum Heat Engines and Quantum Batteries

Capabilities of energy storage and processing devices can perhaps be increased by taking advantage of quantum mechanics. Energy content of a classical battery scales linearly with its mass. Dr. Özgür Müstecaplıoğlu and his students have recently proven that a quantum battery can store energy proportional to the square of its mass. The increase is due to work value of quantum information. Such quadratic increase can be especially advantageous for light weight electric batteries or for batteries in space applications. Moreover, quantum energy resources are clean and non-volatile and can handle such quadratic enhancement safely. In addition, they proposed quantum engines, nanoscale or smaller quantum Otto and Carnot engines to harvest such quantum energy resources. These can be fabricated on chips and can be used to harvest energy more efficiently than classical engines. Their designs are heavily inspired from light harvesting systems and reaction centers in biology and can be used for enhanced quantum photovoltaics. They can be considered as quantum steam engines and can be as revolutionary as a classical steam engine.



Nanoparticle and gelation stabilized functional composites

Thermal Management of Lithium Ion Batteries

The popularity of Li-ion cells in various applications increases everyday due to their high specific energy and specific power. They also offer volume and mass advantage in high power applications. However, compactness of Li-ion battery packs gives rise to safety issues due to potential overheating. Dr. Rıza Kızılel and his students are evaluating Li-ion batteries for high-power Li-ion cells/packs under stressful or abusive conditions. They are aiming to prevent the propagation of thermal runaway in a single cell or adjacent cells. Investigations on high pulse power discharges while preserving sufficiently uniform cell temperature is the aim of their studies. Microchannel heat exchangers are being coupled with the Li-ion batteries in order to increase the cycle life of the battery packs.

Energy Efficiency Map of Turkey

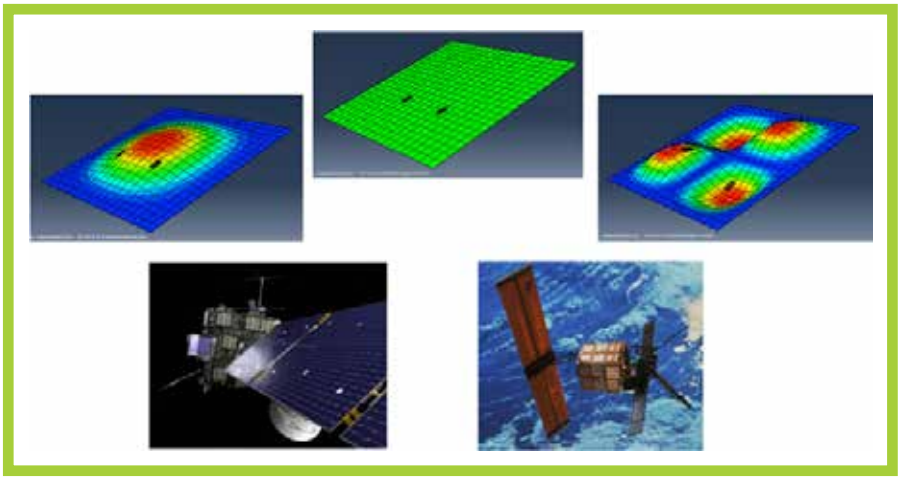
Energy efficiency stands out as an important issue especially regarding supply security, economic development and competitiveness on the one hand, and maintaining the balance between environment and sustainability as well as making important gains in all these issues on the other. Turkey should aim for more efficient use of energy resources, development of deliberate policies of energy security, diversification of energy resources, and development of new technologies. Therefore, Dr. Şuhnaz Yılmaz Özbağcı, Dr. Belgin San Akça, Dr. Metin Türkay and their students thoroughly reviewed the national and international scholarly literature and primary materials on energy efficiency and conducted both national and international benchmarking analyses regarding energy efficiency. Quantitative analyses were conducted for comparisons paving the way for future qualitative research in this field. Leading authorities in the industrial sector, academy, and civil society organizations were contacted and in-depth interviews were carried out.

Energy Harvesting with Smart Materials

In the past two decades, technological advances in electronics have enabled an exponential growth in the use of portable and mobile electronic devices. The miniaturization of these electronic devices has led to a huge reduction in power consumption while leaving each device to carry its own conventional battery with a finite life span. The finite life span of batteries causes unexpected problems and limits the usability of these devices. So, the main motivation of the energy harvesting methodologies is to use renewable energy (solar, thermal, wind) for recharging batteries.

Dr. İpek Başdoğan and her students are using piezoelectric materials for energy harvesting on plate-like structures. The piezoelectric materials have large power densities and can be used as vibration energy harvesters in different structural forms. The most common form of piezoelectric energy harvesters are the 1D cantilever structures where the modeling is very easy however applications are quite limited. Objects for marine aerospace, and automotive applications are mainly composed of plate-like structures and the piezoelectric materials can be easily attached to the surface of these structures. For that reason, they are working on the energy harvesting capabilities of plate-like structures and investigating the power generation performances of different piezoelectric materials.

Simulations and applications of energy harvesters



OUR MAIN MOTIVATION FOR DEVELOPING ENERGY HARVESTING TECHNOLOGIES IS TO USE RENEWABLE ENERGY (SOLAR, THERMAL, WIND) FOR RECHARGING BATTERIES.

Synthesis of Energetic Boron Compounds

Energetic materials are used as ignitors in airbags, solid fuel in rockets and missiles, and in flares. Boron has the third highest heat of combustion value per weight among all elements. However, due to formation of glassy viscose B_2O_3 layer on the boron particles at elevated temperatures, the diffusion of oxygen to the unreacted boron surfaces is almost completely inhibited. Because of the kinetic hindrance, the combustion performance of pure boron in air does not exceed 69%. This can be significantly improved by addition of oxidizers such as PN (potassium nitrate), AP (ammonium perchlorate) or elements such as Mg, Al in pure form or as compound. For example ignitors in a car's airbags are made of a mixture of Boron and PN powders (mass ratio 1:3) whereas AlB_{12} is used as solid propellant in meteor missiles.

Prof. Mehmet Somer and his students are studying the combustion behavior 1:3 blends (1 B-based Material: 3 PN) of nano-Boron, B-95 (boron powder of purity of 95 wt. %), B-92, B-86, AlB_2, AlB_{12}, MgB_2 and $AlMgB_{14}$. In the present calorimetric set-up the combustion experiments are restricted to compounds with heat of combustion values up to 2000 cal/g. Therefore the combustion experiments with pure oxygen using elemental boron could not be conducted, so far, as the heat of combustion of pure boron is almost seven times (14.1 kcal/g) as much as the allowed limit. For this purpose a new special chamber (bomb) will be used which will allow the investigation of the combustion behavior of practically all energetic materials.

PhD & Master Students

PhD Students

Volkan Balcı Elucidation of Structure-Performance Relationships in Supported Metal Catalysts Coated with Phosphonium Type Ionic Liquids

Chemical and Biological Engineering

Reza Sheikhsarmast Mokhtarpoor Joint Probability Density Function Modeling of Turbulent Reacting Flows

Mechanical Engineering

Yasin Karadağ Optofluidics with Liquid Droplets on a Superhydrophobic Surface

Physics

Derya Aydın Investigation of Anti-icing Properties of Bitumen Incorporating Functional Particle Stabilized Emulsion Composite

Chemical and Biological Engineering

Aytaç Denk Turkey's Energy Efficiency Map

International Relations

Navid Solati Interaction of Hydrogen with Single and Multilayer Graphene

Chemistry

İbrahim Şahin Development of Nickel-Based Catalysts as a Cheap Alternative to Ruthenium-Based Counterparts for the Production of Hydrogen from Ammonia

Chemical and Biological Engineering

Haret Türkeri Large Eddy Simulation/ Probability Density Function (LES/PDF) Modeling of Turbulent Reacting Flows

Mechanical Engineering

Mehdi Aas Optofluidic Lasers with Droplet Resonators

Physics

Ramazan Oğuz Canıaz Cracking of Asphalt to Lighter Fractions using Hot and Compressed Water

Chemical and Biological Engineering

Aylin Yardımcı Turkey's Energy Efficiency Map

International Relations

Mohammad Panahi Development of Nitrogen Doped Graphene and Carbon Nitrides

Chemistry

Melike Babucci Investigation of Structural Factors Determining the Applicability Limits and Performance of Imidazolium-Type Ionic Liquid Assisted Catalysts

Chemical and Biological Engineering

Burak Bal Tackling a Critical Problem in Hydrogen Storage through a Multi-scale Modeling Approach: Crack Propagation in the Presence of Hydrogen Embrittlement

Mechanical Engineering

Kubra Bilici Tantalum Oxynitride Based Photoanodes and their Photoelectrochemical Activities

Chemistry

Mustafa Uğur Arıdoğan Vibration-Based Energy Harvesting On Thin Plates with Integrated Piezoelectrics

Mechanical Engineering

Özge Deniz Bozkurt Glycerol Etherification

Chemical and Biological Engineering

Mahza Barzgar Bismuth Vanadate Photoanodes and Their Photoelectrochemical Activities

Chemistry

Sonia Mobassem Investigating Electrochemical Activities of Nitrogen Doped Graphene

Chemistry

Ehsan Saryloo Marine Microalgae Selection and Culture Conditions for Biodiesel Production

Chemical and Biological Engineering

Yasemin Yar Utilization of Nanoparticles in Polymerization Reactions

Materials Science and Engineering

İlknur Eruçar Modeling High Performance Mixed Matrix Membranes

Chemical and Biological Engineering

Ayşegül Bayat Development of Catalysts for Hydrocracking

Chemical and Biological Engineering

Yaprak Özbakır Development of Novel Lab-on-a-chip Optofluidic Waveguides and Flow Manipulation Methods Using Advanced Materials and Fabrication Techniques

Chemical and Biological Engineering

Master of Science Students

Ezgi Erdem Morphological Properties of Pt-Cu Nanoalloys by Density Functional Theory

Chemical and Biological Engineering

Feriha Eylül Saraç Development of Graphene Oxide Based Supercapacitors

Materials Science and Engineering

Mohammedreza Khodabaksh Nanosheets of Perovskite Type Layered Oxides with Optical and Photocatalytic Properties

Materials Science and Engineering

Enes Buz Utilization of Quantum Dots in Polymerization Reactions

Materials Science and Engineering

Şansım Bengisu Barım Preparation of Carbon Aerogel Supported Pt-Cu Nanoalloys by Supercritical Deposition for Fuel Cell Applications

Chemical and Biological Engineering

Navid Solati Effect of Different Subsurface Metals on Hydrogen Storage Properties of Graphene

Chemistry

Elif Kocaman Development of a Catalytic Technology for Liquid Fuel Production from Light Hydrocarbons

Chemical and Biological Engineering

Samira Fatma Kurtoğlu Utilization of Industrial Wastes as Catalysts for the Production of Hydrogen From Ammonia

Chemical and Biological Engineering

Aysim Gülde Kublay Mixed-Integer Non Linear Mathematical Modeling Approach on Renewable Energy Investment Decisions; Turkey's Energy Efficiency Map

Industrial Engineering

Shabrina Virta Inmas Joint Probability Density Function (JPDF) Modeling of Stratified Premixed Flames with Detailed Chemistry

Mechanical Engineering

Mustafa Eryürek Hydrogen Gas Sensor Based on a Polymer Optical Microdisk Resonator

Optoelectronics and Photonics Engineering

Ersan Özelci Optofluidic Microlasers Based on Non-Radiative Energy Transfer in Surface-Supported Liquid Microdroplets

Optoelectronics and Photonics Engineering

Gamze Yılmaz Assessing Potential of Zeolite Imidazolate Framework Membranes in CO_2 Separations Using Molecular Simulations

Chemical and Biological Engineering

Yeliz Gürdal Atomically Detailed Models for Adsorption, Diffusion and Separation of Noble Gas Mixtures in Metal Organic Frameworks

Chemical and Biological Engineering

Tuğba Nur Öztürk Molecular Modeling of Porous Coordination Networks for Flue Gas Separation

Computational Sciences and Engineering

Aydın Özcan Predicting Behaviour of Gas Mixtures in Nanopores Using Pure Gas Data

Chemical and Biological Engineering

Cantay Çalışkan The Success Behind Renewable Energy: A Comparative Analysis of Germany, the United Kingdom, Brazil and Turkey; Turkey's Energy Efficiency Map

International Relations

M. Tahir Kılavuz Turkey's Energy Efficiency Map

International Relations

Buğra Bayık Piezoelectric Energy Harvesting on Plate Like Structures

Mechanical Engineering

GRADUATES

Deniz Şanlı (PhD) Nanostructured Composites of Silica Aerogels with Polymers for Thermal Insulation

Chemical and Biological Engineering

Hasan Şıldır (PhD) Modeling, Optimization and Control of an Industrial Hydrocracker

Chemical and Biological Engineering

İbrahim Şahin (MSc) Hydrocracking of Heavy Vacuum Gas Oil with Zeolite Supported Ni-W Oxide Catalysts

Chemical and Biological Engineering

Metin Karayılan (MSc) Effect of Synthesis Parameters on Thermal and Optical Properties of Silica Aerogels for Thermal Insulation

Chemical and Biological Engineering

Aslı Akçay (MSc) Effects of Structural Changes in Ionic Liquid Cation on Performance of Ionic Liquid-Assisted Catalysts

Chemical and Biological Engineering

Volkan Balcı (MSc) Effects of Structural Changes in Ionic Liquid Anion on Performance of Ionic Liquid-Assisted Catalysts

Chemical and Biological Engineering

INFRASTRUCTURE

- Nanovak Plasma Enhanced Chemical Vapor Deposition (PECVD)
- Applied Separations Supercritical Fluid Extraction System
- Atomic Layer Deposition System by Ultratech
- Q500 TGA with H-Res
- Parr Bomb Calorimeter
- Labconco Laminar Flow
- Agilent GC/MS System
- AutoChem II 2920 Chemisorption Analyzer
- MKS Cirrus 2 Mass Spectrometer
- Bruker Vertex 80v FTIR Spectrometer
- Harrick Insitu FTIR Cell
- Bruker Platinum ATR Diamond Cell
- Micrometritics HPVA II High Pressure Volumetric Analyzer
- Hiden Analytical QGA Mass Spectrometer
- MBraun MB SPS Compact Solvent Purifier
- Agilent 7890A Gas Chromatograph
- FID/TCD Chromatography Detector
- Teledyne Isco Model 500D Syringe Pump (2 pieces)
- Thermocraft 3-Zone Furnaces
- Flow Controllers
- Carbolyte 200 D Tubular Furnace
- Schlenck Line Vacuum Inert Gas Manifold
- Sicco Dessicator
- Newport QE/IPCE Measurement Kit and Accessories
- LCS-100 Solar Simulator
- VSP-300 Potentiostat/Galvanostat
- Nabertherm L-150T3SN Furnaces
- PSI 25L Flat Panel Photobioreactor
- Biostat 5LBioreactor
- Elga Purelab Flex Di-ionized Water Purifier
- Labconco Glove Box 220
- ThorLabs Optic Table
- High Voltage Amplifier
- Lock-in Amplifier
- Oscilloscope
- Function Generator
- Nabertherm Tubular Furnace (Split & 3-Zone)
- Frequency Response Measurement System
- Memmert Ovens
- Vacuum-Ovens
- Witeg Ultrasonic Water Bath
- JSR Chiller (13 L)
- Chiller (8 L)
- Benchmark Incu Shaker 10 L Orbital Shaker
- Benchmark BenchrockerTM3D 3D Shaker
- Ika Rw 20 Set Mechanical Mixer
- Memmert Inc 108 CO2 Incubator
- Witeg Wac-60 Autoclave

OUTREACH

KUTEM provides support for a wide variety of outreach activities ranging from education of undergraduate students in various energy related projects to providing scholarships to students in developing countries to attend conferences. The following outreach activities were supported between 2012 and 2014:

KUTEM Seed Funding

KUTEM offered seed grants to faculty members to initiate research projects in the energy field. Six projects involving 14 faculty members from different disciplines were funded.

- Tackling a Critical Problem in Hydrogen Storage through a Multi-scale Modeling Approach: Crack Propagation in the Presence of Hydrogen Embrittlement (Dr. Demircan Canadinç)
- Piezoelectric Energy Harvesting on Plate-like Structures (Dr. İpek Başdoğan)
- Computational Screening of Porous Coordination Networks as CO_2 Separation Membranes (Dr. Seda Keskin)
- Sustainable Bioenergy Production from Algae (Dr. Halil Kavaklı, Dr. Yeliz Utku Konca, Prof. Mehmet Somer)
- Development of Silver Chalcogenide Sensitized Solar Cells (Dr. Uğur Ünal, Dr. Funda Yağcı Acar)
- Energy Efficiency Map of Turkey (Prof. Metin Türkay, Dr. Şuhnaz Yılmaz Özbağcı, Dr. Belgin San Akça)

US Climate Efforts and Greening Energy

The U.S. Secretary of Energy Dr. Ernest Moniz visited KUTEM on 22 November 2013 and met with faculty members and students. He was interviewed by a student journalist from KU official news magazine KULE, and delivered a speech on "U.S. Climate Efforts and Green Energy". He shared his views on the major problems that the world is facing to meet the increasing energy demand and on how to combat climate change.

When China meets Turkey "All About Energy" Conference

In partnership with Fudan University, KUTEM supported a conference "When China Meets Turkey: Energy Matters," which was held in Koç University on 5-6 December 2012. The conference was intended to mark not only the growing partnership between Fudan and Koç Universities, but also an occasion to celebrate 2012 the Year of China in Turkey, The session topics were: "The Business of Energy" (delivered in a keynote address), "Developments in Energy Technologies", "Investment Opportunities in Energy", "Environmental Aspects of Energy Production", and "The Global Resource: Collaboration and Competition". As a platform for exchange, the conference served to emphasize the importance of academic and business initiatives in the energy realm between China and Turkey – all in the context of a globalized world. After the first day of the Conference, a one day "Poster Session and Competition" with the theme of "Energy Technologies" was organized and 30 successful graduate students from various universities in Turkey presented their posters.

Solar Energy for World Peace

KUTEM supported the International Conference on "Solar Energy for World Peace" which took place in Istanbul Convention Center on August 17-19, 2013. The conference brought together most prominent scientists (among them 4 Nobel prized colleagues) working in the field of solar energy problems, materials and devices. KUTEM provided scholarships to several students (especially from Africa and Middle East as well as Middle and South Asia) which covered the costs of registration, travel and accommodation.

Energy Seminars

A number of seminars on energy were given at Koç University by prominent academicians from all around the world.

- Optimization of Cultivation Parameters in Photobioreactors for Microalgae Cultivation, Martin Trtilek, President and CEO of Photon Systems Instruments
- Potential Methods for Sustainable Hydrogen Production, Prof. Dr. İbrahim Dinçer, Acting President for TÜBİTAK-Marmara Research Center
- Role of Nanoscale in Energy Research, Prof. Dr. Turgut M. Gür, Executive Director of the DOE-EFRC funded Center on Nanostructuring for Efficient Energy Conversion (CNEEC) at Stanford University

Biodiesel Production from Waste Oil from Koç University Cafeteria

As part of the ChBi 402 – Chemical and Biological Engineering Laboratory course, the students carried out experiments in KUTEM Biofuels Laboratory in the Fall 2014 semester to produce biodiesel from waste cooking oil provided by the Sustainable Campus Organization at Koç University. The students investigated the factors affecting the quality of the biodiesel.

Production of Biogas from Organic Wastes

KUTEM is giving support for the activities of the Environment Student Club at Koç University to develop technologies to produce biogas from manure. A large digester was constructed by the students just outside the Engineering Building. A small laboratory scale unit was also set-up at KUTEM in Biofuels Lab where more controlled experiments are being carried out by the students.

TÜBİTAK Formula G- Solar Car Race

KUTEM provided support to the Racing Team consisting of graduate and undergraduate students from various disciplines to construct a solar car for participating in the TÜBİTAK Formula G- Solar Car Race. The team successfully managed to finish the race.

Development of a Biofuels Platform in Istanbul for Renewable Energy

KUTEM is supporting the efforts to establish a biofuels platform in Istanbul for renewable energy. This is a project which is being funded by Istanbul Development Agency and managed by Dr. Halil Kavaklı. The project focuses primarily on using microalgae as the biomass source to obtain hydrocarbon fuels. The research is being carried out in the photobioreactors at the Biofuels Laboratory at KUTEM. The workshops carried out as part of the platform development are bringing together many scientists from Turkey and abroad working primarily on algal technologies.

PUBLICATIONS

2014

1. A. Angi, D. Sanli, C. Erkey and O. Birer, "Catalytic Activity of Copper (II) Oxide Prepared via Ultrasound Assisted Fenton-Like Reaction", Ultrasonics Sonochemistry, 21, 2, 854-859 (2014).
2. R. O. Caniaz and C. Erkey, "Process Intensification for Heavy Oil Upgrading Using Supercritical Water", Chemical Engineering Research and Design, 92, 10, 1845-1863 (2014).
3. D. Sanli and C. Erkey, "Demixing Pressures of Hydroxy-Terminated Poly (dimethylsiloxane)-Carbon Dioxide Binary Mixtures at 313.2 K, 323.2 K and 333.2 K", The Journal of Supercritical Fluids, 92, 264-271 (2014).
4. E. Özelci, M. Aas, A. Jonáš and A. Kiraz, "Optofluidic FRET Microlasers Based on Surface-Supported Liquid Microdroplets", Laser Physics Letters, 144, 1-6 (2014).
5. A. Jonáš, B. Yalizay, S. Akturk and A. Kiraz, "Free-Standing Optofluidic Waveguides Formed on Patterned Superhydrophobic Surfaces", Applied Physics Letters, 104, 1-4 (2014).
6. E. Ozelci, M. Aas, A. Jonas and A. Kiraz, "Miniature Droplet-Based FRET Lasers Stabilized by Superhydrophobic Surfaces", CLEO: Science and Innovations, 124, 1-2 (2014).
7. S. Anand, D. McGloin, H. Bayraktar and A. Kiraz, "In-vitro and in-vivo Biolasing of Fluorescent Proteins Suspended in Liquid Microdroplet Cavities", Lab on a Chip, 14, 3093-3100 (2014).
8. S. Acikgoz, M. M. Demir, E. Yapasan, A. Kiraz, A. A. Unal and M. N. Inci, "Investigation of the Spontaneous Emission Rate of Perylene Dye Molecules Encapsulated into Three-Dimensional Nanofibers via FLIM Method", Applied Physics A, 174, 1867-1875 (2014).
9. A. Akcay, V. Balci and A. Uzun, "Structural Factors Controlling Thermal Stability of Imidazolium Ionic Liquids with 1-n-Butyl-3-Methylimidazolium Cation on γ-Al_2O_3", Thermochimica Acta, 589, 131-136 (2014).
10. S. M. Toker, D. Canadinc, A. Taube, G. Gerstein and H.J. Maier, "On the Role of Slip – Twin Interactions on the Impact Behavior of High-Manganese Austenitic Steels", Materials Science and Engineering A, 593, 120-126 (2014).
11. R. Mokhtarpoor, H. Turkeri and M. Muradoglu, "A New Robust Consistent Hybrid Finite-Volume/Particle Method for Solving the PDF Model Equations of Turbulent Reactive Flows", Computers & Fluids, 105, 39-57 (2014).
12. M. Muradoglu and G. Tryggvason, "Simulations of Soluble Surfactants in 3D Multiphase Flow", Journal of Computational Physics, 274, 737-757 (2014).
13. N. Shahraki and M.Turkay, "Analysis of Interaction among Land-Use, Transportation Network and Air Pollution Using Stochastic Nonlinear Programming", International Journal of Environmental Science and Technology, 11, 8, 2201-2216 (2014).
14. A. Ozcan and S. Keskin, "Effects of Molecular Simulation Parameters on Predicting Gas Separation Performance of ZIFs", Journal of Chemical Technology & Biotechnology, 90, 9, 1707-1718 (2014).
15. T. Ozturk and S. Keskin, "Computational Screening of PCNs for Adsorption and Membrane-based Gas Separations" Journal of Physical Chemistry C, 118, 25, 13988-13997 (2014).
16. G. Yilmaz, A. Ozcan and S. Keskin, "Computational Screening of ZIFs for CO_2 Separations", Molecular Simulations, 41, 9, 713-726 (2015).
17. I. Erucar and S. Keskin "Molecular Modeling of MOF-based Mixed Matrix Membranes", Current Organic Chemistry, 18, 18, 2364-2380 (2014).
18. G. Yilmaz and S. Keskin, "Molecular Modeling of MOF and ZIF-filled MMMs for CO_2/N_2 Separations", Journal of Membrane Science, 454, 407-417 (2014).
19. A. Uzun and S. Keskin "Site Characteristics in Metal Organic Frameworks for Gas Adsorption", Progress in Surface Science, 89, 56-79 (2014).
20. I. Erucar, T. Manz and S. Keskin, "Effects of Electrostatic Interactions on Gas Adsorption and Permeability of MOF Membranes", Molecular Simulation, 40, 557-570 (2014).
21. M. Arici, O. Z. Yesilel, S. Keskin and O. Sahin, "Gas Adsorption/Separation Properties of Metal Directed Self-Assembly of Two Coordination Polymers with 5-nitroisophthalate", Journal of Solid State Chemistry, 210, 280-286 (2014).
22. H. Erer, O. Z. Yesilel, M. Arici, S. Keskin and O. Buyukgungor, "2D-3D Polycatenated and 3D-3D Interpenetrated Metal–Organic Frameworks Constructed from Thiophene-2,5-Dicarboxylate and Rigid Bis(Imidazole) Ligands" Journal of Solid State Chemistry, 210, 261-266 (2014).
23. S. Kanyas, D. Aydin, R. Kizilel, A. L. Demirel and S. Kizilel, "Nanoparticle and Gelation Stabilized Functional Composites of an Ionic Salt in a Hydrophobic Polymer Matrix" PLoS ONE, 9, 2, 1-14 (2014).

24. H. Sildir, Y. Arkun, A. Ari, I. Dogan and M. Harmankaya, "Economic Model Predictive Control of an Industrial Fluid Catalytic Cracker", Industrial and Engineering Chemistry Research, 53, 45, 17696-17704 (2014).

25. H. S. Casalongue, J. Benck, C. Tsai, R. K. B. Karlsson, S. Kaya, L. G. M. Pettersson, F. Abild-Pedersen, J. K. Norskov, H. Ogasawara, T. Jaramillo and A. Nilsson, "Operando Characterization of an Amorphous Molybdenum Sulfide Nanoparticle Catalyst during the Hydrogen Evolution Reaction", Journal of Physical Chemistry C, 118, 50, 29252-29259 (2014).

26. U. Aridogan, I. Basdogan and A. Erturk, "Analytical Modeling and Experimental Validation of a Structurally Integrated Piezoelectric Energy Harvester on a Thin Plate", Smart Materials and Structures, 23, 4, 1-13 (2014).

27. U. Aridogan, I. Basdogan and A. Erturk, "Multiple Patch-Based Broadband Piezoelectric Energy Harvesting on Plate-Based Structures", Journal of Intelligent Material Systems and Structures, 25, 14, 1664-1680 (2014).

2013

1. T. N. Ozturk and S. Keskin, "Predicting Gas Separation Performances of PCNs Using Atomistic Simulations", Industrial and Engineering Chemistry Research, 52, 49, 7627-7639 (2013)

2. A. Uzun and S. Keskin. "Site Characteristics in Metal Organic Frameworks for Gas Adsorption", Progress in Surface Science, 89, 56-79 (2013).

3. M. Aas, A. Jonáš and A. Kiraz, "Lasing in Optically Manipulated, Dye-doped Emulsion Microdroplets", Optics Communication, 290, 183-187 (2013).

4. Z. Ulker, I. Eruçar, S. Keskin and C. Erkey, "Novel Nanostructured Composites of Silica Aerogels with a Metal Organic Framework", Microporous and Mesoporous Materials, 170, 11, 352-358 (2013).

5. G. Eris, D. Sanli, Z. Ulker, S. Bozbag, A. Jonas, A. Kiraz and C. Erkey, "Three-Dimensional Optofluidic Waveguides in Hydrophobic Silica Aerogels via Supercritical Fluid Processing", The Journal of Supercritical Fluids, 73, 28-23 (2013).

6. D. Sanli, and C. Erkey, "Bubble Point Pressures and Densities of Hexamethyldisiloxane–Carbon Dioxide Binary Mixture Using a Constant Volume View Cell", The Journal of Supercritical Fluids, 74, 52-60 (2013).

7. I. Erucar, G. Yilmaz and S. Keskin, "Recent Advances in Metal Organic Framework-based Mixed Matrix Membranes", Chemistry - An Asian Journal, 8, 8, 1692-1704 (2013).

8. Y. Gurdal and S. Keskin "Predicting Noble Gas Separation Performance of Metal Organic Frameworks Using Theoretical Correlations", Journal of Physical Chemistry C, 117, 10, 5229–5241 (2013).

9. I. Erucar and S. Keskin, "High CO_2 Selectivity of an Amine-Functionalized Metal Organic Framework in Adsorption-based and Membrane-based Gas Separations", Industrial and Engineering Chemistry Research, 52, 9, 3462-3472 (2013).

10. S. Keskin, "Gas Adsorption and Diffusion in a Highly CO_2 Selective Metal Organic Framework: Molecular Simulations", Molecular Simulation, 39, 1, 14-24 (2013).

11. G. Günay, O.Z. Yesilel, C. Darcan, S. Keskin and O. Buyukgungor, "Synthesis, Crystal Structures, Molecular Simulations for Hydrogen Gas Adsorption, Fluorescent and Antimicrobial Properties of Pyrazine-2,3-Dicarboxylate Complexes", Inorganica Chimica Acta, 399, 19-35 (2013).

12. F. Semerci, O. Z. Yesilel, H. Soylu, S. Keskin and O. Buyukgungor, "A Two-Dimensional Photoluminescent Cadmium(II) Coordination Polymer Containing a New Coordination Mode of Pyridine-2,3-Dicarboxylate: Synthesis, Structure and Molecular Simulations for Gas Storage and Separation Applications", Polyhedron, 50, 314-320 (2013).

13. F. Semerci, O. Z. Yesilel, S. Keskin, C. Darcan, M. Tas and H. Dal, "Construction of Homo- and Heterometallic-Pyridine-2,3-Dicarboxylate Metallosupramolecular Networks with Structural Diversity: 1D T5(2) Water Tape and Unexpected Coordination Mode of Pyridine-2,3-Dicarboxylate" (CrystalEngComm) 15, 1244-256 (2013).

14. Y. Karadag , A. Jonáš, I. Kucukkara and A. Kiraz, "Size-Stabilization of Surface-Supported Liquid Aerosols Using Tapered Optical Fiber Coupling", Optics Letters, 38, 5, 793-795 (2013).

15. H. Sildir, Y. Arkun, B. Cakal, D. Gokce and E. Kuzu , "Plant-Wide Hierarchical Optimization and Control of an Industrial Hydrocracking Process", Journal of Process Control, 23, 9, 1229–1240 (2013).

FUNDINGS – AWARDS

EU 7TH FRAMEWORK				
	Project	**Director**	**Granted (TL)**	**Duration**
1	**NANOINSULATE - Nano-Technology Based Vacuum Insulation for Building Envelopes**	CAN ERKEY	1,309,329	2010-2014
2	**COMMOF - Composite Membranes with Metal Organic Frameworks for High Efficiency Gas Separations**	SEDA KESKİN AVCI	287,790	2010-2014
	TOTAL		**1,597,119**	

MINISTRY OF INDUSTRY				
	Project	**Director**	**Granted (TL)**	**Duration**
1	**Development of Nanostructured Materials Warm to the Touch**	CAN ERKEY	147,194	2014-2016
	TOTAL		**147,194**	

ISTANBUL DEVELOPMENT AGENCY				
	Project	**Director**	**Granted (TL)**	**Duration**
1	**Development of a Biofuels Platform in Istanbul for Renewable Energy**	HALİL KAVAKLI	1,017,371	2014-2015
	TOTAL		**1,017,371**	

TÜBİTAK				
	Project	**Director**	**Granted (TL)**	**Duration**
1	**Filtered Density Function Modeling of Turbulent Reacting Flows**	METİN MURADOĞLU	253,890	2011-2014
2	**Development of Novel Lab-on-a-chip Optofluidic Waveguides and Flow Manipulation Methods Using Advanced Materials and Fabrication Techniques**	ALPER KİRAZ	195,268	2013-2015
3	**Development of Waste Battery Disposal and Recovery Technologies**	METİN TÜRKAY	442,978	2009-2014
4	**Modifying Hydrogenation and Nitrogenation Capabilities of Graphene**	SARP KAYA	436,500	2014-2017
5	**Unlocking the Potential of Zeolite Imidazolate Frameworks as Membranes for Carbon Dioxide Separations Using Molecular Simulations**	SEDA KESKİN AVCI	152,793	2011-2013
6	**Transparent Vacuum Insulation Panels for Thermal Insulation in Refrigerators**	CAN ERKEY	370,015	2010-2014
7	**Investigation and Development of Metal and Metaloxide Microdisk Resonator Inflammable Gas Sensors**	ALPER KİRAZ	327,550	2011-2014
8	**Investigation of Structural Factors Determining the Applicability Limits and Performance of Imidazolium-Type Ionic Liquid Assisted Catalysts**	ALPER UZUN	292,500	2013-2016
9	**Development of Tunable Microlasers Based on Optically Stretched Microdroplets Suspended in a Microfluidic Chip**	ALPER KİRAZ	261,560	2011-2013
10	**Design, Manufacturing and Membrane, Electrode and Catalyst Development and Testing for Polymer Electrolyte Membrane Fuel Cells Operating at Ultra-Low Stoichiometric Flows in the Anode**	RIZA KIZILEL	276,530	2014-2017
11	**Improving the Selectivity of Polymeric Membranes Using Metal Organic Frameworks as Fillers**	SEDA KESKİN AVCI	145,300,00	2014-2016
12	**Development of Nickel-Based Catalysts as a Cheap Alternative to Ruthenium-Based Counterparts for the Production of Hydrogen from Ammonia**	ALPER UZUN	467,629	2014-2016
13	**The Effect of Cell Dimensions and Number of Electrode Layers on the 20Ah Li-ion Cells Used in Electric Vehicles and the Improvement of Thermal Management System by Microchannel Heat Exchanger**	RIZA KIZILEL	530,312	2015-2018
14	**Improving Methane Storage Performance and Stability of Cu-BTC MOF Using Ionic Liquids**	ALPER UZUN	512,068	2015-2018
	TOTAL		**4,664,893**	

Tüpraş				
	Project	Director	Granted (TL)	Duration
1	**Development of Laboratory Scale Hydrocracking Reactors and Catalysts for Hydrocracking**	CAN ERKEY	300,900	2010-2013
2	**Real-time Optimization and Control of a Hydrocracker Unit**	YAMAN ARKUN	140,358	2010-2013
3	**Elimination of Ice Formation on Functional Coatings**	SEDA KIZILEL	346,070	2011-2014
4	**Industrial Application of Real Time Optimization and Control to Fluid Catalytic Cracking**	YAMAN ARKUN	138,000	2012-2014
5	**Development of Hydrocracking Catalysts**	CAN ERKEY	180,000	2013-2016
6	**Simultaneous Maximization of Octane Number and Productivity in Isomerization Plant**	SEDA KESKİN AVCI	60,000	2013-2015
7	**Modeling and Optimization of Entire Refinery**	METİN TÜRKAY	192,000	2013-2015
8	**Modeling, Optimization and Control of an Industrial Diesel Hydroprocessing Plant**	YAMAN ARKUN	140,033	2013-2015
9	**Development of Alternative Fuel Additives and Determination of Their Fuel Competitiveness**	ALPER UZUN	172,320	2013-2016
10	**Development of a Technology to Produce Light and Mid-Distillates by Olefin Oligomerization**	ALPER UZUN	189,480	2014-2017
	TOTAL		**1,859,161**	

KOÇ UNIVERSITY SEED RESEARCH FUND				
	Project	**Director**	**Granted (TL)**	**Duration**
1	**Development of a Collaborative Research Program on Methane Storage Combining Experiments with Atomic Simulations: I. Simulations (CH4toGo-I) – II. Experimental (CH4toGo-II)**	SEDA KESKİN AVCI ALPER UZUN	258,000	2014-2016
2	**Electrochemical CO_2 and CO Reduction to Make Methanol Fuel**	SARP KAYA	39,543	2014-2016
3	**Energy Efficiency Map of Turkey**	ŞUHNAZ YILMAZ ÖZBAĞCI METİN TÜRKAY BELGİN SAN AKÇA	30,000	2012-2013
4	**Computational Screening of Porous Coordination Networks as CO_2 Separation Membranes**	SEDA KESKİN AVCI	54,474	2012-2014
5	**Tackling a Critical Problem in Hydrogen Storage through a Multi-scale Modeling Approach: Crack Propagation in the Presence of Hydrogen Embrittlement**	DEMİRCAN CANADİNÇ	68,624	2012-2014
6	**Development of Silver Chalcogenide Sensitized Solar Cells**	HAVVA YAĞCI ACAR UĞUR ÜNAL	67,924	2012-2014
7	**Piezoelectric Energy Harvesting on Plate-like Structures**	FATMA İPEK BAŞDOĞAN	55,944	2012-2014
8	**Sustainable Bioenergy Production from Algae**	YELİZ UTKU KONCA HALİL KAVAKLI MEHMET SOMER	65,525	2012-2014
	TOTAL		**640,034**	

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