Rovira i Virgili University

Department of Chemical Engineering
(http://www.etseq.urv.es/9deg/ca/6-home.html)

Project Proposals for the

NEU-URV Student Exchange

April-July 2014
Project #1

Title: Understanding complex systems using big data

Supervisors: Roger Guimerà Manrique & Marta Sales-Pardo

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Description:

Technological advances during the last fifteen years have boosted our capacity to generate and store data in many areas of science and business. Indeed, 90% of the world’s stored data has been generated in the last two years, and the availability of such large quantities of data (for example time-resolved geo-location of mobile devices or usage data of social networks) is changing the way we think about crisis response, social mobilization, marketing, and intelligence.

Big data is a particularly relevant opportunity for the study of complex systems such as cells, ecosystems or economies. In complex systems, non-linear interactions among the many components that comprise the system give rise to macroscopic behaviors that cannot be explained by looking at individual components alone. Traditionally, the analysis of complex systems was constrained by the limited information available from the different components (and layers of components) comprising the system (for example, metabolites and proteins in cells, species in ecosystems, and people and institutions in economies). The availability of unprecedented highly detailed data on these systems opens the door to significantly advance our understanding of their behavior, and of how this behavior evolves in time. With large amounts of data we now have the possibility to uncover correlations and patterns that will enable us to build predictive models of these systems.

The goal of our research is to contribute, from the perspective of statistical mechanics, new tools and methods for the analysis and modeling of large-scale datasets.

This project will involve computational work, thus students selecting this project should have an interest in programming.

Positions: 2

Project #2

Title: Self-assembling polymers for novel proton transport membranes

Supervisors: Marta Giamberini

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Description:

In the last 40 years, there has been a growing interest toward the "hydrogen economy", that is a system where hydrogen is in charge of energy delivery and acts as an energy carrier (like electricity) and not as a primary energy source (like coal or oil). This could be a possible solution to the huge energy problems caused by the disappearance of fossil fuels. On the other hand, hydrogen needs to be produced by an energy consuming method, stored and finally used as fuel in a fuel cell to deliver electric energy when needed.

As far as hydrogen production is concerned, the idea of using solar energy to perform water splitting, according to the reaction:

\[ 2\text{H}_2\text{O} \rightarrow 2\text{H}_2 + \text{O}_2 \]

is currently under development. The energy required for this reaction can be supplied by sunlight, but requires the use of a dye-sensitized solar cell, as water does not absorb the electromagnetic radiation emitted by the sun to promote water splitting in a kinetically facile way. This process can be combined with the reduction of carbon dioxide to carbohydrates, and is generally referred to as "artificial photosynthesis". As presented in the international conference “TOWARDS GLOBAL ARTIFICIAL PHOTOSYNTHESIS. Energy, Nanochemistry & Governance”, the artificial photosynthesis project has the category of a global research project comparing or even overtaking the Human Genoma project. The two red-ox half-reactions involved in water splitting must take place in two different compartments so that hydrogen and oxygen gases can be stored in different containers. For this reason, a water-splitting device has to include in a single cell the following components: a light harvesting device, a water-oxidation catalyst, a proton-reduction catalyst and a proton-exchange membrane (PEM). The separation of the anodic and cathodic compartments through a PEM is crucial in order to separate efficiently \( \text{H}_2 \) and \( \text{O}_2 \) as well as to prevent short-circuiting of the cell. Moreover, in such a device the PEM should be capable of resisting quite severe conditions of pH and red-ox potentials.

Fuel cells are a kind of electrochemical device that converts chemical energy directly into electrical energy. They can be divided into five major categories: alkaline, phosphoric acid, solid oxide, molten carbonate and proton exchange membrane. Proton exchange membrane fuel cells (PEMFC) work at relatively low temperature (about 80 °C), have high power density, can vary their output quickly to meet shifts in power demand and are suitable for automobile applications. In PEMFCs the electrolyte is constituted by a polymer membrane, able to conduct protons, which is sandwiched between two electrodes. They, in turn, contain Pt-based catalysts that allow the oxidation and reduction reactions to take place. Among PEMFCs, we can find hydrogen fuel cells and direct methanol fuel cells (DMFC).

In DMFCs, the fuel is directly methanol; this entails several advantages over fuel cell systems based on hydrogen and compressed natural gas, as methanol can be simply transported and applied under room temperature and atmospheric pressure by pumping from existing gasoline infrastructures without an external compressor or refrigeration equipment. This makes the volume of DMFCs as small as possible.

Furthermore, methanol has the highest hydrogen-to-carbon ratio among alcohols, thus giving the highest energy generation and the least carbon dioxide emissions; in addition, methanol is miscible with water: as a consequence, DMFCs can be fueled with different concentrations of a methanol aqueous solution. Besides, methanol can be obtained through biomass and is more environmentally friendly than gasoline since it breaks down quickly in the environment. The ideal membrane to be used in a DMFC should resist to relatively high temperatures, transport protons efficiently, be an insulator to
electrons, act as barrier between the anode and cathode, possess good mechanical strength and be inexpensive.

The membranes currently used as PEM are far away to be considered optima with regard to their performance; therefore, the development of new proton exchange membranes is a topic of permanent interest. In this project we tackle this problem by preparing membranes based on self-assembling columnar side-chain liquid-crystalline polymers which lead to the formation of biomimetic ionic channels. These channels contain basic atoms (oxygen or nitrogen) to interact with protons thus allowing their transport across the membrane.


Positions: 2

1. The first one deals with the synthesis and characterization of columnar side-chain liquid-crystalline polymers. This internship is addressed to students with an Organic Chemistry background. We offer the possibility of working with the classical methodology of the organic chemistry synthesis, as well as with techniques such as $^1$H and $^{13}$C NMR, Fourier-transform infra-red spectroscopy (FTIR), polarized optical microscopy (POM), differential scanning calorimetry (DSC), and small and wide-angle X-ray diffraction (XRD).

2. The second one is focused on the preparation and assessment of PEMs based on columnar side-chain liquid-crystalline polymers. In this case, the internship is addressed to students with Applied Chemistry or Chemical Engineering background. The student will have the possibility to work with membrane preparation techniques, microscopic techniques (environmental and conventional scanning electron microscopy -E-SEM, SEM, confocal microscopy-CM, atomic force microscopy-AFM) and contact angle measurements, as well as with XRD and POM; moreover, permeability tests will be eventually performed.

Project #3

Title: Molecular simulation of the self-assembly of micellar systems

Supervisors: Allan Mackie

Contact: allan.mackie@urv.cat

Research Group: Molecular Simulation (I. Complex Systems) (http://www.etseq.urv.es/ms/)

Description:
Many of the new applications in biomedicine and nanotechnology, such as the design of miniaturised chemical processes and new functional products, are based on the possibility of controlling the formation of structures and dynamic processes at the mesoscale and processes at the micro- and even nanoscale. The understanding and control of the mechanisms that relate the functionality and supramolecular structure with the microscopic composition of the constituents is the cornerstone for developing new intelligent materials having a strong impact in, for instance, biomedical applications, selective drug delivery, tissue repair, molecular recognition, and many others. The development of new industries in Europe and the USA, oriented to the production and application of products with high added value based on cutting edge R+D, is key to maintaining the competitiveness of our industries on an increasingly competitive global stage.

\[ \mu_1^{\theta} \quad N=1 \\
X_1 \]

To be able to deliver the products and processes previously portrayed requires the development of fast predictive tools capable of exploring the capacities of molecules in the formation of superstructures and functionality at the nanoscopic scale, and which avoids the need for slow and costly empirical research in a vast universe of compounds and different thermodynamic conditions. Molecular simulation allows this virtual exploration to be undertaken in a fast and cheap way, and should serve as a guide for the indispensable experimental exploration in a final stage.

In this project, the student is asked to participate in one of our ongoing projects where we are seeking to understand and control the mechanisms that make micelles choose a particular size and shape. Micelles form when surfactants are found under conditions that make the aggregates of several tens or even hundreds of surfactants spontaneously self-assemble. Even though such systems are widely used in many industries, models which are able to quantitatively link the surfactant molecular structure to the final micellar solution properties are lacking. We propose to use both Monte Carlo molecular simulation as well as a Self Consistent Single Chain Mean Field Theory in order to explore and better understand these systems.

Positions: 1

Project #4

Title: Simulation of bioethanol production plants

Supervisors: Laureano Jiménez Esteller & Gonzalo Guillén Gosálbez

Contact: laureano.jimenez@urv.cat / gonzalo.guillen@urv.cat


Description:
This offer deals with the development of realistic process simulation models in order to compare the potential economical and environmental impact of some process design alternatives for bioethanol production processes.

The analysis is based on the combined use of process simulation tools (i.e. SuperPro Designer and Aspen Hysys), optimization software (i.e. Matlab, GAMS) and environmental impact assessment. The aim of the method is provide an optimal process design of different biofuels production plants that simultaneously accounts for the maximization of the Net Present Value (NPV) and the minimization of the environmental impact (EI).

The specific objectives of the project are:
1. Development of a realistic model for the production of bioethanol.
2. Search for alternatives processes in order to improve performance.
3. Search for data for environmental and economic assessment of the plant.

It is recommendable the student to be familiar with modelling tools (Aspen Hysys, SuperPro…).

Positions: 1

**Project #5**

**Title:** Cost-benefit analysis of energy efficiency measures in buildings

**Supervisors:** Dieter Boer & Laureano Jiménez Esteller

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**Research Group:** Sustainable Computer Aided Process Engineering, SUSCAPE (http://www.etseq.urv.es/suscape/)

**Description:**

The energy consumption of buildings has an important contribution on the total energy demand. Thus, improving their energy efficiency is necessary for the reduction of greenhouse gas emissions. It is among the priorities established in the energetic plans established by national governments and the EC.

In this context the integration of energy storage in different forms shows a significant potential. In order to evaluate the effect of different materials and technologies it is necessary to establish models which represent the thermal behavior of different types of buildings and storage. In the frame of this work we will review the most important types of materials used. This includes both classical insulation materials, but also phase change materials, which may increase the thermal inertia of buildings. In order to evaluate the cost-benefit of them it is necessary to gather data on their environmental impact and their economic cost. This work forms part of a research project on the improvement of energy efficiencies in buildings.

The specific objectives of the project are:

1. Review of most relevant insulation and phase change materials for building application.
2. Review the life cycle assessment for the case study of a cubicle with different materials.
3. Evaluate the cost of different design alternatives for the case study of a cubicle with different materials.

It is recommendable the student to be familiar with modelling tools (Engineering Equation Solver, Excel, GAMS …).

**Positions:** 1

**Period:** May-Jul 2014.
Project #6

Title: Preparation and characterisation of bioconjugates from cyclodextrin nanosponges

Supervisor: Alex Fragoso

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Research Group: Nanobiotechnology and Bioanalysis Group, NBG (http://www.etseq.urv.es/nbg/)

Description:

The student will work on the preparation and characterisation of bioconjugates from cyclodextrin nanosponges (CDNS). These are hypercrosslinked polymers having a spherical shape prepared by reaction of cyclodextrins and a bifunctional reagent. Azide-terminated CDNS will be initially reduced to form aminated particles that will be further reacted with antibodies or enzymes using different bioconjugation strategies. The encapsulation properties of these nanomaterials will be studied using model compounds and the particles will be characterised by microscopy and spectroscopic techniques.

Positions: 1

Project #7

Title: Photocatalytic water splitting

Supervisors: Dr. Francesc Medina / Dr. Sandra Contreras / Dr. Ivan Dafinov

Contact: francesc.medina@urv.cat

Research Group: Heterogeneous Catalysis Group, CATHETER (http://www.etseq.urv.es/catalis/)

Description:

Photocatalytic water splitting is a general term used for the production of hydrogen from water. In this process, water is dissociated into its elements (H₂ and O₂) using either natural or artificial light. The objective of this project is the synthesis of Mo-alloys supported on TiO₂ catalysts and the study of their effects on the production of hydrogen using artificial light lamps from UV to visible light. The synthesis of the Mo-alloys could be performed at the Department of Chemical Engineering a la Northeastern University under the supervision of Prof. Elizabeth Podlaha-Muphy, whereas the Mo-Alloys supported catalysts and the activity of these materials for the production of hydrogen by splitting of water could be carried out at the Chemical Engineering Department of the Rovira i Virgili University (Tarragona, Spain), under the supervision of Prof. Medina.

Positions: 1

Project #8

**Title:** Encapsulation of food aromas using protein-polysaccharide complexes  
**Supervisors:** Dr. C. Güell and Dr. M. Ferrando  
**Contact:** carme.guell@urv.cat; montse.ferrando@urv.cat  
**Research Group:** Food Innovation & Engineering (FoodIE)  

**Description:** The use of protein-polysaccharide complexes as emulsifiers has been proven feasible in the encapsulation of lemon essential oil. This project will study the encapsulation of a pizza aroma (on a sunflower oil base) using whey protein-polysaccharide (Arabic gum or maltodextrin) complexes to produce oil-in-water (O/W) emulsions by premix membrane emulsification. The final encapsulation will be obtained by adding the wall forming material and drying with a spray-drier. An asymmetric screening experimental design will be used to select the experimental plan to study the effect of the following factors: oil fraction, type of complex, type of membrane and type of wall forming material. Size of emulsions and microcapsules will be characterized by laser diffraction, oil encapsulation efficiency by chemical extraction methods and morphology of the microcapsules by scanning electron microscopy. Depending on the candidate interests, the project will continue studying the volatile release of the microcapsules or their thermal stability under actual process conditions.

**Positions:** 1  
**Period:** May-Jul 2014.
Title: Long-range correlations in liquid water

Supervisors: Josep Bonet Avalos http://www.researcherid.com/rid/A-2761-2010
Contact: josep.bonet@urv.cat
Research Group: Molecular Simulation (II Polymers and Interfaces) (http://www.etseq.urv.es/ms/)

Description:
Water is one of the most fascinating substances in nature and its intriguing properties are still matter of intense debate [1,2]. Supercooled bulk water presents long range correlations as well as long-time decays proper of glassy systems, due to the strong correlated hydrogen bonding interactions. These properties are particularly sensitive to the confinement and are assumed to be of about 1nm long [3,4].

Many questions arise around the anomalies presented by liquid water like such as the maximum density of liquid water at about 4ºC, the decrease of viscosity under pressure, the minimum of the isothermal compressibility or the minimum of the specific heat Cp, both at atmospheric pressure. Some explanations are based on the idea that two different morphologies coexist for liquid water even at ambient temperature [5], which would be reminiscent of the conjectured liquid-liquid phase transition in the deep supercooled region [1] if it may exist [2].

By means of standard molecular dynamics simulations [6] we aim at studying the local morphology of liquid water in a wide range of temperatures (from ambient down to supercooled) at atmospheric pressure. We will introduce the appropriate order parameter and its correlations to identify and characterise the instantaneous local water morphology and its transformation by lowering the temperature. The main objective is to identify the structures causing the rise of the structure factor S(k) as k ->0 and describe its dynamics.

The ideal candidate
She or he should have some knowledge of a programming language, preferably C (or Fortran) or Matlab, to deal with the data treatment after the simulation. The student will learn the use of DL_POLY and the analysis of the data to obtain physical information from the simulation.

References

Positions: 1
Title: Development of an advanced protein immobilization system

Supervisors: Lluis Masip

Contact: lluis.masip@urv.cat

Research Group: Bioengineering and Bioelectrochemistry Group (http://www.etseq.urv.es/BBG/)

Description:

Students will work on the development of a novel protein immobilization system with a wide range of applications in the field of biosensors. Students will learn basic molecular biotechnology techniques in order to produce proteins in bacteria (from cloning of the gene of interest in an expression vector to producing the protein in a bacterial host) and their isolation and purification.

Positions: 1

Project #10

Prof. Anton Vernet, Characterization and use of alginate microparticles for PIV

The student will learn the Particle Image Velocimetry (PIV) technique for visualization of fluid flow. This technique needs a specific type of microparticles that are synthesized in our research group (ECoMMFiT). The student will work in the characterization of the particles and will use them to obtain flow patterns in some laboratory flow systems

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Project #11

Prof. Clara Salueña, Hydrodynamic simulations of flow in granular media (silo flow).

The student will learn how from a simple model of granular media arise complex hydrodynamic-like equations for the flow. The simulations will be based on the use (as user) of an existing code for granular media with the final objective of reproducing the behavior of particulate materials flowing in usual geometries typical of real applications

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