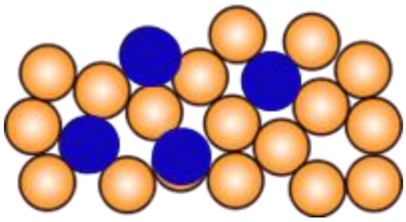
CEA Saclay –Service de Physique de l'Etat Condensé (SPEC) (page web)
Laboratoire *SPHYNX* (page web)

PROPOSITION DE STAGE/THESE 2020

TAKING UP THE CHALLENGE OF THE GLASS TRANSITION BY OPTICAL MANIPULATIONS OF MOLECULES.



Schematic view of optically active molecules (in blue) pinned by their interaction with a well chosen light, and immersed in a glass forming liquid insensitive to the light (orange).

According to the Nobel Prize awardee P.W. Anderson "The deepest and most interesting unsolved problem in solid state theory is probably the nature of glass and the glass transition". This sentence reflects the fact that we still do not know if glasses are a true thermodynamic phase of matter or, on the contrary, if they are just out of equilibrium liquids which have become too viscous to flow on human time scales. Finding the answer to this seemingly simple question is hampered by the fact that, when decreasing temperature, the relaxation time of glass forming liquids becomes so large that one cannot rely onto the experimental techniques used to evidence standard thermodynamic phase transitions (e.g. liquid/gas transition or liquid/crystal transition). By using a totally new approach we aim at unveiling the nature of the glass transition, which is of great importance both for fundamental physics and for applications, since glasses play an increasing role in modern technologies (e.g. in optical fibers for communications, in photovoltaic devices, or in airplanes fuselages).

More precisely, we have just built an experiment corresponding to the "ideal thought experiment" proposed recently by some theorists, so as to unveil the presence or the absence of a true thermodynamic glass transition. In this experiment a fraction of molecules, randomly chosen in space, is pinned and one monitors the response of the rest of the liquid: if this pinning of a small fraction of molecules changes the global dynamics of the liquid, this means unambiguously that an order was present before establishing the pinning field, even though the extremely complex nature of this order had made it impossible to evidence by standard experimental tools. The approach that we have built involves: i) designing the optically sensitive molecules; ii) building an optical setup allowing the realize pinning in the well-chosen liquid; iii) comparing the experimental results to the theoretical predictions. The internship and/or the thesis consists in working onto the improvment and the exploitation of this experiment.

This project is a collaboration gathering all the required expertise between physicists, chemists, and theoreticians working at CEA Saclay –near Paris- and in the University of Montpellier. The internship and/or the thesis will mainly take place in the NIMBE/LIONS and SPEC/SPHYNX laboratories in the CEA center of Saclay. We are looking for a candidate who, by relying onto the expertise available in the laboratories, really wants to invest herself/himself onto this project by providing us his/her skills in experimental physics (mainly optics, and dielectric spectroscopy).

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PROPOSITION DE STAGE/THESE 2020

THERMALLY CHARGING IONIC SUPERCAPACITOR WITH VERTICALLY ALIGNED CARBON NANOTUBE ELECTRODES

Supercapacitors store electrical charge via electrical double-layer (EDL) formation at the electrolyte/electrode interface. They are characterized by their faster charging/discharging times compared to batteries, but suffer from lower energy (charge) density. Therefore, supercapacitors are used in quick power delivery and low-voltage applications such as in volatile memory backups. While conventional supercapacitors are charged using an external voltage source, Thermally Charged Ionic Supercapacitors (TISC) take advantage of the thermoelectric effects inside the electrolyte (thermos-electro diffusion) and at the electrolyte/electrode interface (EDL) to charge itself using 'heat.' As such TISC made with highly thermoelectric ionic liquids is considered as an alternative technology for waste-heat recovery applications. The performance of TISC's depends on key parameters; notably, the induced thermoelectric voltage and the specific capacitance of the electrodes. One possibility to improve the latter is to increase the electrode surface area by nanostructuration. For example, vertically aligned carbon nanotubes (VACNT) based materials are a promising candidate to build an efficient supercapacitor. However, the precise electrochemical and physical processes in TISCs are still unclear; and it is yet to be determined if TISC can become competitive against other thermos-electrochemical energy storage technologies.

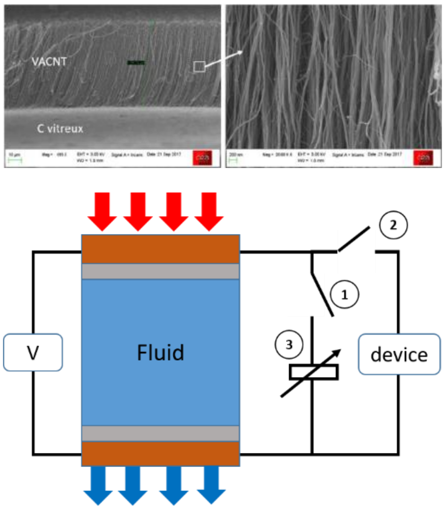

Figure 1 (Top) SEM images of vertically aligned carbon nanotubes grown on glassy carbon surface (courtesy of LEDNA/NIMBE/IRAMIS/CEA). (Bottom) A schematic illustration of a thermally chargeable ionic supercapacitor. ① Switch connecting a (charging) resistance ③ to the TISC cell. ② Switch connecting the electronic device to the TISC.

The proposed internship at SPHYNX/SPEC/IRAMIS (UMR 3680 CEA-CNRS) and LEDNA/NIMBE/IRAMIS mainly experimental: the characterization of thermoelectric properties (thermoelectric voltage and capacitance) of TISC devices using VACNT electrodes in combination with the mixtures of ionic liquids and organic solvents. The student will also participate in the electrode elaboration. More specifically, he/she will perform thermoelectrical and capacitance measurements, implementation of automated data acquisition techniques and analysis of the resulting data obtained. The student will also acquire hands-on experience in basic electrochemical characterization techniques (cyclic voltammetry and impedance measurements). The electrode synthesis will be conducted at LEDNA, using their 1-step process developed for the direct and controlled growth of vertically aligned and dense carbon nanotubes. In addition to these principal responsibilities, the student will also have the opportunity to learn materials characterization techniques such as Scanning Electron Microscopy, X-ray Photoelectron Spectroscopy and Transmission Electron Microscopy (at LEDNA). For a motivated candidate, participation in the numerical investigation of ionic liquid – electrode interactions through Monte Carlo simulation technique can also be envisaged. A successful internship may be converted to a PhD research in where a systematic comparison of thermoelectric data to the morphology (nanotube arrangements, lengths, diameter/density distribution etc.) will be investigated in order to understand the physical and electrochemical mechanisms of the thermoelectric energy conversion in complex liquids in ionic supercapacitors.

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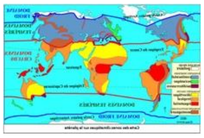
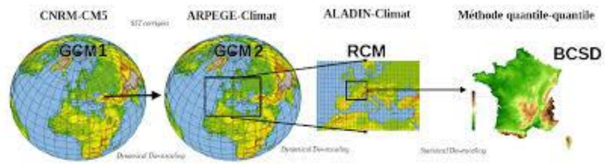
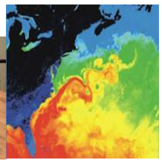
PROPOSITION DE STAGE/THESE 2020

PEUT-ON SIMULER LE CLIMAT SUR UN ORDINATEUR PORTABLE ?

Les gaz à effet de serre produits par l'activité humaine influencent le climat de la Terre. Pour comprendre et prédire cette influence, la communauté scientifique utilise entre autre des simulations numériques du système climatique. Ce dernier est multi-composant, et implique une gamme pharaonique d'échelles : par exemple, la simulation de l'athmosphère (une des composantes du climat) requière en principe la prise en compte de toutes les echelles entre celle des ouragans (100 km) et celles à laquelle l'énergie est dissipée (0.1 mm), soit une gamme d'échelle de 10^{11}. Cette gamme d'échelle est inaccessible aux plus grands ordinateurs existant actuellement, qui n'ont ni assez de mémoire, ni assez de CPU pour traiter un tel nombre de degré de libertés.

Par ailleurs, le traitement complet de toutes les échelles du problème cache un gaspillage énorme : 90 pour cent des ressources informatiques sont monopolisées par le traitement des toutes petites échelles (inférieur à 1m), alors que seules les grandes échelles intéressent les scientifiques, le climat à l'échelle d'une maison n'ayant que peu de pertinence.

La solution actuelle adoptée par les climatologues est d'introduire des « modèles de turbulence », grâce auquels l'influence des petites échelles est paramétrisée via des loi empirique, au prix de l'introduction de paramètres ajustables. Ainsi, un modèle de climat moderne en comporte plus de 100. L'ajustement de ces paramètres empiriques est alors un enjeu majeur, qui n'est pas encore résolu.

Dans ce stage, nous proposons une nouvelle approche, qui consiste à considérer toute la gamme des échelles, mais en raréfiant le nombre d'échelles prises en compte au fur et à mesure que l'on descend en taille. Le modèle correspondant est sans paramètre ajustable, et peut etre simulé sur un ordinateur portable.

Le but de ce stage est de tester les limites de ce modèle, en l'appliquant sur une représentation simplifiée de l'atmosphère. La majeure partie du travail impliquera des simulation en Matlab, sur un petit ordinateur. Des comparaison avec des resultats numériques issus de simulations de toute la gamme d'échelle seront également éffectuées.

Le cœur de ce stage est numérique, mais des développements théoriques sur théorie de la turbulence via le formalisme multi-fractal et les ondelettes pourront être effectués. Ce stage sera encadré par B. Dubrulle (CNRS). Le sujet stage requiert une solide formation de physicien, en particulier en physique nonlinéaire, ainsi qu'un goût prononcé pour le numérique. Il pourra éventuellement déboucher sur une thèse sur une thématique voisine.

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