Post doc subject: **Investigation of interfacial properties in nano-reinforced polymers**

Post doc Advisor:

- Fahmi BEDOUI, MCF-HDR
  Roberval laboratory, FRE CNRS-UTC 2012
  +33 (0)3 44 23 45 28, fahmi.bedoui@utc.fr

Context of the study:

The emergence of practical synthesis and assembly of a diversity of nano-structured systems provides the opportunity to develop optimal designs for specific challenging applications. The simultaneous advances in quantum mechanics based multiscale atomistic and continuum scale simulations provides new opportunities to guide the experiment with realistic simulations on how the compositions and structures can be manipulated to achieve optimum properties at minimum cost.
Indeed, these opportunities are widely recognized, with international competition, especially regarding the development of new devices and tools for exploring and exploiting the unusual physical aspects of nano-structured materials in such technological fields, as energy, electronics, biology, pharma, water. environment. These developments are particularly important for tackling the challenging human needs of energy, water, health, and environment. However, there remain tremendous challenges in predicting and measuring the properties exploitable for the *end user*. They depend on a complex sequence of elementary phenomena that cross the length scales ranging from atomic scales (*Ångström*) governed by the QM and atomistic MD, transition through scales dominated by microstructure, ending with the macroscale (cm and beyond) of the end user system. The consequence is that it is not yet possible to optimize engineering systems. We must start to integrate into the design modeling and optimization of the salient interactions at each scale to include how they impact the larger scales. *The current empirically based engineering approach toward developing new nano-based systems must be enriched and led by modeling coupled with synthesis and experimental characterization. In this proposal, we will focus on polymer-based nano-structured systems and the opportunities offered by nano-reinforced polymers for developing novel materials that are strong and smart. Thus, our main objective here is to answer the question:* ***How can connecting length scales hierarchically from first principles to practical engineering systems lead to stronger and smarter materials, capable of responding both to human needs and overcoming human challenges?***

Post doc description:

The emphasis in the development of reinforced polymers has been on increasing ultimate properties, such as stiffness and load. Nano-reinforced materials were the answer to almost all of those requirements. Recent experimental works nanocomposites made, at constant volume fraction, of mixture of silica nano-particles (size ranging from 500 to 15 nm) and poly(methyl methacrylate) polymer[17, 18] demonstrate the dependency of a materials' macroscopic response (elastic and viscoelastic for instance) on the size of the reinforcing nano-particles (figure 1). Recent molecumlar dynamics simulations in similar material configuration of silica nano-partricles (3 and 4 nm) reinforced PMMA confirmed the mechanical properties dependency on the particle size.
Experimental data along with molecular dynamics simulation provided the evidence that unlike common composite materials, nano-reinforced polymers macroscopic properties do not only depend on the volume fraction and heterogeneity shape ratio, but also on the size of heterogeneous species. The results provided new insight into the interaction modes taking place at key material length scales for small and simple combination of O-H terminated silica and PMMA polymer. Such configuration,

although interesting, is still limited compared to the many combinations we can imagine in terms of particle properties (type, size, surface treatment) and the polymeric matrix.

If size effects are proven to enhance mechanical properties, no evidence, as far as the proposal participants know, of such effects on other phenomena such as magnetic or piezoelectric properties are reported. We target to study size effects on thermal, mechanical and piezoelectric properties of nano-reinforced materials by using **superparamagnetic** nano-particles with **different sizes** and **surface chemistry** mixed with thermoplastic (polyvinylidene difluoride as example for its piezoelectric behavior) and elastomers (Polydimethylsiloxane as example of hyperelastic material). As such, combination of NP size, surface chemistry and polymer matrix could be used as leverage to enhance the desired properties (mechanical, electrical or magnetic) and accelerate the development of many devices from Néel effect based sensor[3] to tunable mechanical properties through magnetic fields[4] or thermo-electric energy harvester[5]. In addition, the tuning the electrical properties of the fabricated nano-composites will be addressed, opening the way to the development of new electroactive-based high performance sensors.

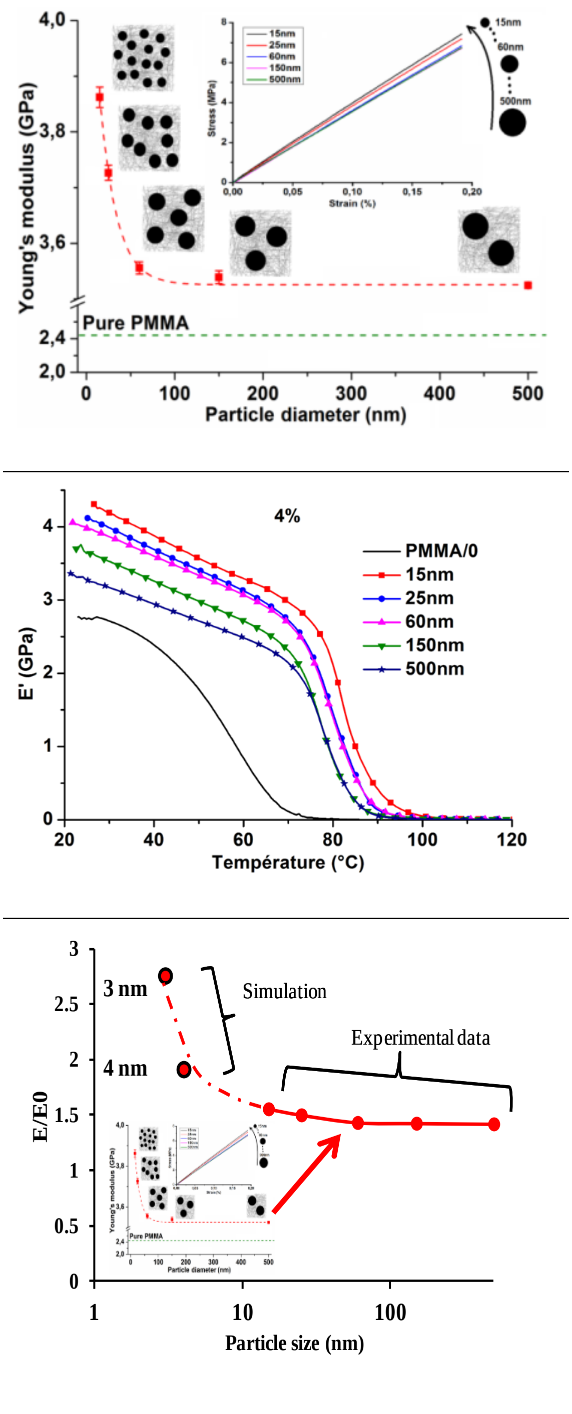

Figure 1: Experimental(elastic[1] and viscoelastic properties) and simulation[2] size effect evidence on elastic modulus of 4% silica-PMMA composites

Given the tremendous options we encounter in terms of nanoparticle compositions, sizes, surface treatment along with the multitude of available polymers; it is impossible to perform experimental screening of all plausible combinations in a reasonable timeframe. Thus, we want to guide these developments using rational and optimal design. For nanocomposites aimed at engineering applications we require the development of new paradigm allowing us to identification in advance of experiment the best candidate materials, sizes, surface treatments, and polymer chemistry to attain maximum performance at minimum cost. Therefore, the main objectives of this project will be to perform an *a priori* screening using first-principles based molecular dynamics of superparamagnetic NPs within a variety of polymer matrices to establish interfacial properties, properties dependencies on NP size, and system composition, leading to improved mechanical and electrical response. Therefore fast-screening and cost-effective development methodology suited for larger systems covering larger combinations is desired. Such approach will be based on breakthrough modeling and simulation technologies developed by MSC/Caltech.

This prostdoc proposal is meant to understand the mechanism underlying the extraordinary properties offered by nano-particles and therefore help guide the experiments. Particular attention will be given to explore the interfacial properties between the NP and the surrounding polymer. New developed methodologie (figure 2) allows to access to precious mechanical-related information at this specific lengh-scale. The role of the postdoc is to confirm such approach on a chosen configurations NP-Polymer and extend this approach to explore other properties such as thermal, electric, piezo electric , …

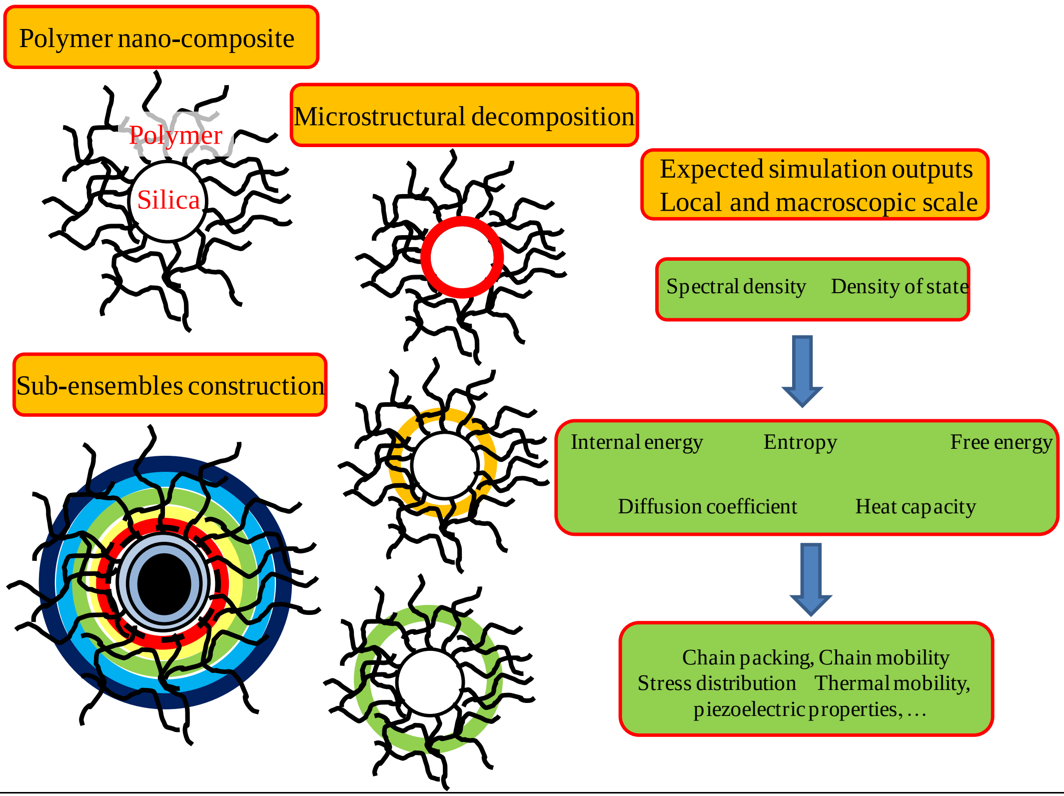

Figure 2: Schematic representation of interfacial thermodynamic properties.

Candidate's profile:

- Strong experience with atomistic simluation softwares like LAMMPS, Shrodinger, … is mandatory,
- .Experience with nano-composites development is required
- Interest and ability to work in an interdisciplinary research environment and across disciplines; teaming with material scientists, engineers and theoretical chemists.
- Good English communication skills, including development/delivery of presentations to technical and non-technical audiences are required.

- Ability to write coherent and compelling scientific documents

Documents required to apply:

Send to fahmi.bedoui@utc.fr

- Curriculum vitae
- Motivation letter
- At least two references and/or recommendation letters
- A statement of research experience and interests

Location:

Laboratory Roberval UTC-CNRS FRE 2012
Université de Technologie de Compiègne (UTC)
Centre de recherche de Royallieu
BP 20529 Rue Personne de Roberval
60205 Compiègne cedex –France

References:

1. A.S.Blivi, F.Benhui, J.Bai, D.Kondo, and F.Bedoui. Polymer Testing 2016;56:337-343.
2. Bedoui F, Jaramillo-Botero A, and Goddard-III WA. Engineering Mechanics Institute Conference 2019 - EMI-Caltech 2018;June 18-21, 2019, Pasadena, CA, USA.
3. Lenglet L and Motte L. Neel Effect: Exploiting the nonlinear behaviour of superparamagnetic nanoparticles for applications in life sciences up to electrical engineering: Elsevier, Amsterdam, Kidlington, Cambridge, 2018.
4. Mitsumata T and Ohori S. Polymer Chemistry 2011;2(5):1063-1067.
5. Zhao W, Liu Z, Sun Z, Zhang Q, Wei P, Mu X, Zhou H, Li C, Ma S, He D, Ji P, Zhu W, Nie X, Su X, Tang X, Shen B, Dong X, Yang J, Liu Y, and Shi J. Nature 2017;549:247.