Université de technologie de Compiègne – Thesis proposal

Part 1: Scientific sheet	
Thesis proposal title	***Nanocomposite behavior modeling by molecular dynamics approach: case of multifunctional materials***
PhD grant	Ph.D. Scholarship through LEEGO chair program
Research laboratory	research team: Roberval Laboratory (UTC) and Materials and process Simulation Center (CalTech) web site: https://www.utc.fr/en/research/utc-research-units/mechanics-energy-and-electricity-roberval/
Thesis supervisor(s)	Fahmi Bedoui (UTC) and William A. Goddard (CalTech)
Scientific domain(s)	Chemistry, Physics, Science and technology
Research work	In recent years, the emphasis in the realm of composite materials is no longer just to develop strong materials but now is strong *and* smart materials with enhanced properties (mechanical but also electrical, thermal, optical, etc.). This is quite valuable for many applications in the fields of energy, electronics, environment and health. The now requires development of approaches to combine, in a single composite material, multiple properties (called multifunctional materials). However, the mechanisms for improving each targeted functionality may be at different scales or based on different physics. This can lead to a situation, where reaching optimal performance for one criterion might not guarantee optimal performances for the other properties. Therefore, the objective of this proposal is to develop new materials with multiple and balanced properties. *Given the enormous set of options in terms of materials choice and targeted performances, it is impossible to perform experimental screening of all probable combinations in a reasonable timeframe.* In this context, the innovative aspect of this proposal is to develop a new paradigm based on a **hybrid in-silico and experimental approach** capable of understanding the underlying mechanisms of the drastic enhancement, then predicting macroscopic properties from the very first synthesis steps of composite materials design. Success of this approach would be a **breakthrough** in terms of opening possibilities of **tuning** materials properties toward **combined performance criteria**. Although a large body of literature exists studying composites with improved specific properties, no previous study, to our knowledge, has been reported considering the investigation of simultaneous multiple properties using both modeling and experiment. To showcase our approach, we will focus our study on polymers reinforced with nanoparticles (NPs), (*nano-reinforced polymers)* and target two properties (mechanical and electrical). Due to their high surface-to-volume ratio, NPs, used as nano-fillers, can interact strongly with the polymer, that can lead to drastic enhancement of mechanical (stiffness and ultimate stress) and electrical (piezoelectric) properties. Moreover, because NPs are usually passivated with surfactants, the role of the surfactant/polymer interactions, in addition to that of the size, needs to be integrated into the modeling of the nanocomposite materials through the most advance methodology and validated through carefully designed experiments. In this proposal, we focus on the case of the nano-reinforced PVDF (polyvinylidene fluoride). The electroactive matrix based on PVDF couples mechanical flexibility with interesting electroactive properties. Maghemite NPs with stringent requirements regarding size, surface chemistry and chemical stability will be used as nanofillers. This combination of composite materials will allow us to investigate from both **experimental** and **modeling** approaches the capabilities of ***multi-criteria optimization*** toward ***materials*** with ***enhanced electric and mechanical properties simultaneously***.
Key words	
Requirements	The PhD proposal is joint position between Roberval-UTC and MSC-Caltech. In this regard, the student will spend at least the first months on site at the Materials and Process Simulation Center (MSC) at the California Institute of Technology (Caltech) in Pasadena, CA USA. Required skills:

	Master's degree in materials science or applied physics with emphasis on computational chemistry or chemistry or chemical engineering with an emphasis on materials will be highly desired. Hands on experience with powerful MD simulation tools (LAMMPS, VASP, Jaguar from Schrodinger, Gromacs) are required Advanced English level: writing and speaking. Willing to travel between USA and France during the course of the PhD. To apply please send: CV, motivation letter, and two references willing to send recommendation letters to: Dr. Fahmi Bedoui; fahmi.bedoui@utc.fr Prof. William A. Goddard III; wag@caltech.edu and cc wagoddard3@gmail.com Dr. Andres Jaramillo-Botero; ajaramil@caltech.edu
Starting time	As soon as possible
Location	UTC France and CalTech, USA

Part 2: Job description	
Duration	36 months
Additional missions available	
Research laboratory	Roberval-UTC : materials science MSC-California Institute of Technology: Computational chemistry and applied physics
Material resources	Office, acces to computational facilities et UTC and CalTech,
Human resources	Ph.D
Financial resources	Ph.D. scholorship in France and support allowance when visiting CalTech
Working conditions	
Research project	LEEGO chair
National collaborations	
International collaborations	Materials and Process Simulation Center, California Institute of Technologie.
International cosupervision	Materials and Process Simulation Center, California Institute of Technologie.
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Please contact first the thesis supervisor before applying online on https://webapplis.utc.fr/admissions/doctorants/accueil.jsf