French Polytech network form for PhD Research Grants from the China Scholarship Council

This document describes one of the PhD subjects proposed by the French Polytech network. The network is composed of 15 engineering schools/universities. The document also provides information about the supervisor. Please contact the PhD supervisor by email for further information regarding your application.

Supervisor information	
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PhD information	
Title	Improving mechanical performances of bio-inspired composites for building and construction applications
Main topics regards to CSC list (3 topics at maximum)	Calculation of materials and simulation for design ; Environmental behavior and failure of materials ; Intelligent construction

Required skills in science and engineering	Civil engineering; Mechanics; Computational tools

Subject description (two pages maximum including biblio)

The development of strain-hardening building materials becomes a world concern. Several efforts have been done to provide a higher strength and durability to cementitious materials but nature suggests we can do better. Nature offers numerous examples of very specific natural materials like bioinspired nanocomposites, with unique structure and properties that are under an intensive investigation in basic scientific disciplines. Particularly, nacre represents one excellent representative of the natural bioinorganic material with interesting mechanical properties such as high strength and toughness. Nacre is two-level biocomposite consisting from nanograins of hard mineral aragonite ($CaCO_3$ polymorph) glued with soft biopolymer binders (proteins, polysaccharides). Its mechanical properties are much higher than corresponding properties of the parent materials aragonite. The high resolution imaging techniques showed nano-asperities of the microplatelet tiles that are connected with mineral bridges. In the second, microscale level, these platelets form brick-and-mortar layered structure with thickness of 0.2—0.5 μm (~95% volume fraction) embedded in biopolymer binders (~5%) represented mainly by proteins and polysaccharides This unique combination of inorganic and organic moieties results in interesting mechanical properties, much higher strength and fracture toughness than parent inorganic material aragonite. The tensile strength and Young's modulus of the nacre is in the range of 80−135 MPa and 60−70 GPa (depending on the wet or dry states) which give rise to the tensile toughness of around 1.8 MJ/m^3 calculated by integrating the area underneath the stress−strain curve. Fracture testing showed that the fracture toughness of nacre is about 1.5 kJ/m^2, ~3000 times higher than ~0.5 J/m^2 of pure calcium carbonate. Owing to the extraordinary mechanical properties, nacre is extensively studied experimentally in order to understand the relation between its microstructure and properties, which knowledge can help in a preparation of novel high-strength layered composites. Following experiments various models and mechanisms have been proposed for explaining unusual strengthening in nacre such as small size scale of the building blocks, mineral bridges between nanograins, abrupt steps and nano-asperities on the platelet surfaces, or nanostructured tablets.

In spite of numerous experiments, complete molecular-scale knowledge about the organic-inorganic interface is still not fully achieved. In this context, molecular modelling methods can be an effective tool for revealing mechanisms and interactions responsible for the formation of bioinorganic composite materials such as nacre.

This proposal is aimed to contribute to the mechanistic understanding of the interactions and forces responsible for the formation of bioorganic-inorganic interfaces in nanocomposites of the nacre type at molecular scale by using methods of molecular modeling. Various representative models of biopolymer-aragonite composites will be developed. They will cover surface models of aragonite, lamellae structures, and nanoplatelet mineral grains embedded in the cross-linked polymer matrix. Biopolymers used in the simulations will be based on protein and polysaccharide structures. Molecular simulations will be conducted to describe in details the structure of the interface between aragonite surfaces and biopolymer moiety and the nature of the binding between these two phases. It is expected, that using a systematic approach to the design of the structural models and applying appropriate molecular modeling approach will significantly help to reveal the nature of the interactions between inorganic and biopolymer phases and to the explanation of the unusual mechanical properties of the nacre biocomposite. The achieved results can also help to material scientists in their effort to prepare synthetic organo-mineral composites with specific properties such as nacre has. This novel concept will help to attain the balance between strength, toughness and ductility in order to develop advanced bio-inspired composites and new manufacturing technologies such as 3D printing of cementitious materials. This leads to the development of more abundant and low-cost materials such as cement and concretes.

The main aim *of this project is*

- to contribute to the mechanistic understanding of the interactions and forces responsible for the formation of the bioorganic-inorganic interfaces in nanocomposites of the nacre type at a molecular scale by using methods of molecular modelling including a prediction of their mechanical properties. It is supposed that the surface structure of aragonite microplatelets and chemical nature of biopolymer binder are crucial factors for the formation, stability, and properties of the natural composite nacre. Molecular simulations can help in revealing of the basic interaction mechanisms between parent materials. Further, molecular modelling methods will be also used in the prediction of mechanical properties of the developed representative models based on the structure of the nacre-like bioinorganic composites.

Specific project aims will comprise

- developing and design of the representative structural models of nacre-like composites based on minerals such as aragonite and selected natural biopolymers such as polysaccharides and proteins
- to elucidate structure and chemistry at interfaces of the developed models of bioorgano-inorganic composites with estimation of the adhesion energies between both constituents
- prediction of the mechanical properties (e.g. elastic constants, bulk, shear, Young modulus, stress-strain curves, etc.)
- to find a relation between origin of parent materials, their chemistry, composition, stacking and arrangement in the biocomposite models and the corresponding mechanical properties
- in order to validate developed models (and correct them if necessary) predicted properties will be compared with the available experimental data.