

The Research Group

**General Chemistry**

has the honor to invite you to the public defense of the PhD thesis of

**Yangyang Su**

to obtain the degree of Doctor of Sciences

Joint PhD with Northwestern Polytechnical University

Title of the PhD thesis:

**Investigation of Biological Mineralization Interfaces Applied to a Selected Series of Medical Applications using Experimental and Theoretical Tools**

Promotors:

**Prof. dr. Frederik Tielens (VUB)**

**Prof. dr. Kezhi Li (Northwestern Polytechnical University)**

The defense will take place on  
**Tuesday, May 31, 2022 at 9.00-12.00 h**

The defense can also be followed through a livestream. Please contact yangyang.su@vub.be for more information.

**Members of the jury**

Prof. dr. Frank De Proft (VUB, chair)

Prof. dr. Yue Gao (VUB, secretary)

Prof. dr. Marc Elskens (VUB)

Prof. dr. Jie Kong (Northwestern Polytechnical University)

Prof. dr. Leilei Zhang (Northwestern Polytechnical University)

Prof. dr. Dominique Bazin (Université Paris-Saclay)

Prof. dr. Xueni Zhao (Shaanxi University of Science and Technology)

Prof. dr. Monica Calatayud (Sorbonne Université)

### Curriculum vitae

Yangyang Su obtained her MSc. Degree in Material Engineering with distinction from the Northwestern Polytechnical University (NPU) in 2018, and then continued to her PhD. She started her joint PhD program in General Chemistry at VUB and NPU during 2019 - 2021. Her research was funded by China Scholarship Council and dealt with the study of biomineralization regarding kidney stones by using theoretical and experimental tools. During her PhD she has published 7 peer-reviewed papers in international journals and 2 in draft. She participated at several conferences and has teaching experience at NPU.

### Abstract of the PhD research

Biological minerals normally appeared in the living, including calcium phosphate, calcium oxalate, etc. Our work was chiefly two broad families: a) the bio-coatings modified carbon/carbon (C/C) composites; b) pathological mineralization.

(i) The C/C composites are promising biomaterials in clinic surgery. But their biological inertia, hydrophobicity, carbon particles release extremely restricted further applications. Surface modification is a good way to solve above problems. Hydroxyapatite (HA) is the modified material due to outstanding bioactivity and striking bonding with bone tissues. In our work, HA coating was sprayed on C/C. However, high sprayed temperature led to several coating defects. Thus, we invented a microwave-hydrothermal (MH) method showing fast heating rate, controllable heating temperature, etc., to provide some solutions. The influence of various conditions on mechanical and biological behaviours was studied to analyse the MH reaction mechanism. In comparison, Ca-P solution was the best way to lower sprayed defects. Whilst tuning pH and concentration of complexing agents of Ca-P solution decreased crystal size formed on MH treated coatings, thus forming polka-dot-, cotton-, block-, needle- and rod- like particles. Where, rod-like crystal with good mechanical and biological properties, played a vital role in bone tissue, following the "oriented attachment" and "Ostwald" ripening theories.

(ii) Effect of citrate ion on the calcium oxalates' crystal (mono- and dehydrated forms - COM and COD) morphology was studied by using periodic dispersion corrected density functional theory (DFT-D). Compared with experimental results, citrate ion's inhibiting character on the growth of calcium oxalate at the molecular level, notably the COM. Besides, genetic diseases affecting the metabolism of cysteine and the kidney function occurred cystinuria and cystinosis, thus generating cystine. Recently, the presence of cysteine has been underlined in the case of cystinosis, where two cysteine molecules consisted of cystine connected by a disulfide (S-S) bond. The theoretical and experimental results showed that cystine regarding cystinuria and cystinosis also resulted from the conversion of cysteine, leading to a mixture of cysteine and cystine.