

# Experimental report

13/02/2021

**Proposal:** CRG-2761

**Council:** 4/2020

**Title:** Conformational Change of Bioinspired Polymer Brushes Caused by Specific Capture of Heavy Metal Ion.

**Research area:** Soft condensed matter

**This proposal is a new proposal**

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**Samples:** Silicon  
Phytochelatin

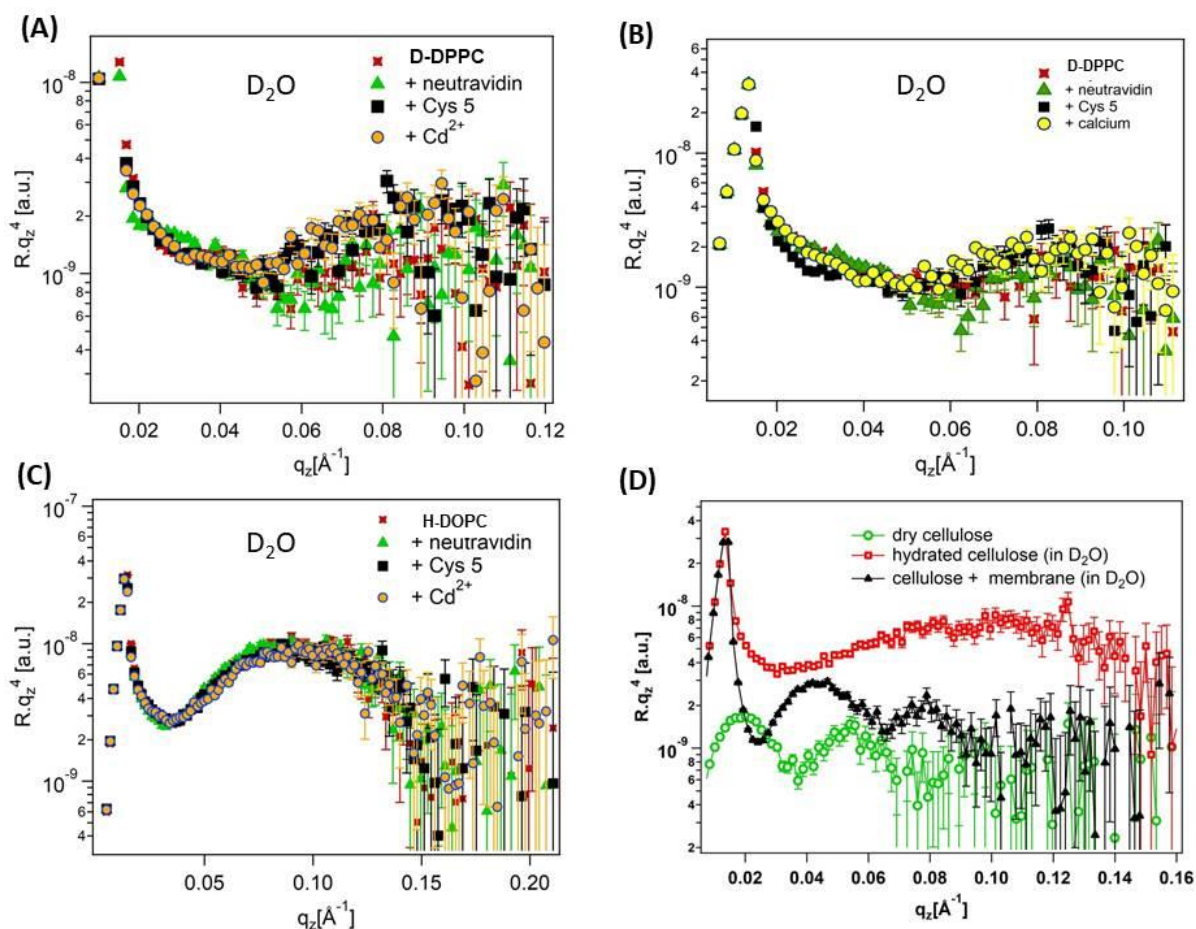
Instrument	Requested days	Allocated days	From	To
SUPERADAM	6	6	04/02/2021	09/02/2021

## Abstract:

To clean up soil and water contaminated with hazardous contaminants using plants, called phytoremediation, relies on the ability of plants to concentrate contaminants from the environment and to detoxify with aid of a protein, phytochelatin (PhyCh). For example, the dissociation constant of PhyCh to  $\text{Cd}^{2+}$  is  $K_d \sim 10^{-13}$  M, which is more than 10 orders of magnitude lower than the commercially used crown ether ( $K_d \sim 10^{-2}$  M). The main aim of the proposed project is to gain deeper insights into conformational changes of PhyCh-inspired polymer brushes at the solid/liquid interface. PhyCh-inspired polymers are grafted onto the surface of a supported membrane via biotin-neutravidin crosslinkers, which enables the precise control of lateral density of polymer brushes. Specular neutron reflectivity experiments at SuperADAM with an outstanding resolution in  $q$  enables us to sensitively detect subtle changes in the thickness, density, and roughness of polymer brushes in the presence of monovalent cations (e.g.  $\text{Na}^+$ ,  $\text{K}^+$ ) and divalent cations ( $\text{Ca}^{2+}$ ,  $\text{Cd}^{2+}$ , etc.)

## Conformational Change of Bioinspired Polymer Brushes Caused by Specific Capture of Heavy Metal Ion.

The Lipid bilayer from vesicle suspension of deuterated lipids (D-DPPC) was deposited on Silicon-block ( $5 \times 8 \times 2 \text{ cm}^3$ ) and incubated solid-liquid measurement cell at  $T \sim 45^\circ\text{C}$  for at least 3 hours prior to NR measurement (red cross, figure 1A). In the next step neutravidin solution was injected into the cell and incubated for 3 hours at room temperature. After rinsing with Tris buffer the NR curve is recorded (green triangles, figure 1A). The later step is repeated for polymer brush Cys 5 (black squares, figure 1A).



**Figure 1:** (A) NR curves of polymer brush Cys 5 coupled to D-DPPC in the presence of  $\text{Cd}^{2+}$  ions and (B) in the presence of  $\text{Ca}^{2+}$  ions. (C) NR curves of polymer brush Cys 5 coupled to DOPC in the presence of  $\text{Cd}^{2+}$  ions. (D) NR curves of polymer supported membrane.

Eventually, the subphase is exchanged with Tris-buffer containing 1 mM  $\text{CdCl}_2$  and NR curve was recorded after 3 hours of incubation at room temperature (yellow circles, figure 1A). The differences between NR curves are very small. However the global shape of the NR curve suggests that the quality of the bilayer is not very good. The same set of experiments were repeated and the final buffer is replaced with Tris-buffer containing  $\text{Ca}^{2+}$  ions (figure 1B). The shift of NR curves toward lower q-values upon addition of extra-layer (e.g. neutravidin, polymer brush Cys 5) indicates the increase in total film thickness. Moreover, after the addition of  $\text{Ca}^{2+}$  ions the NR curve is shifted to higher q-value indicating that the polymer brush is cross-linked by Ca ions. However, the global shape of the NR curve suggests a low bilayer quality. The same set of measurements were repeated with deuterated DPPC is replaced with hydrogenated H-DOPC (figure 1C). The NR curves indicate better bilayer quality but the contrast between different films (neutravidin, Cys 5 and lipid bilayer) is low. At the end of the beam time polymer (cellulose) supported membrane is measured to confirm the possibility of depositing biological membranes on polymer support at macroscopic length scale ( $5 \times 8 \text{ cm}^2$ ) (figure 1D).