



## Study of the interaction of sorbed silver, gold and copper ions with functional groups on hydrolyzed fibroin using Charmm22 force field calculations

Khushnubek Odilbekovich Eshchanov <sup>a, \*</sup>, Mukhabbat Matnazarovna Baltaeva <sup>a</sup>

<sup>a</sup> Department of Chemistry, Faculty of Natural Sciences, Urgench State University, Urgench, Uzbekistan

### ARTICLE INFO

#### Article history:

Received 30 March 2022

Received in revised form 10 May 2022

Accepted 18 May 2022

Available online 28 May 2022

#### Keywords:

Charmm22 force field

Hydrolyzed fibroin ("HF")

Nanoparticles

Coordination bonds

IR spectrum

### ABSTRACT

We studied the sorption of silver, gold, and copper ions into powdered hydrolyzed fibroin derived from silk fibroin fibers. Metal ions sorbed into hydrolyzed fibroin have been found to interact with active functional groups over time. It was hypothesized that the silver and gold ions sorbed into hydrolyzed fibroin would form nanoparticles as a result of the reduction reaction, while the copper ions would form a coordination bond. Charmm22 force field calculations were performed on this basis. The IR spectral results obtained by calculations were compared with the IR spectral results obtained in practice, and it was proved that silver and gold nanoparticles were formed and that copper ions formed coordination bonds with fibroin.

### 1. Introduction

The silk industry produces a large amount of fibrous waste that does not meet the requirements of textiles. One of the important issues is to obtain and use materials with sorption properties from the fibrous waste of natural silk.

Silk fiber consists of fibroin and sericin proteins. Silk fibroin has unique sorption properties. Silk fibroin fiber has the property of sorption of various substances. Sorption of  $Pb^{2+}$ ,  $Mn^{2+}$ ,  $Co^{2+}$ ,  $Cu^{2+}$  ions into Bombyx mori silk fibroin has been studied [1, 2]. The sorption process of  $Pd^{2+}$  ions to silk fibroin has been studied in solutions with the same concentration and mixed ions ( $Pt^{2+}$ ,  $Os^{4+}$ ,  $Ir^{4+}$ ,  $Rh^{3+}$  and  $Ru^{4+}$ ) [3]. The sorption of  $Cs^{+}$  ions into silk fibroin is well studied [4].

Samples in the form of powders with sorption properties derived from silk fibroin can be used for technical purposes and in pharmacy [5, 6]. Powdered fibroin samples can be obtained by hydrolysis of silk fibroin fiber under the action of various reagents. The number of amino- and carboxyl groups increases in the discontinuities of the powder sample obtained [7, 8]. Powdered fibroin pores also contain polyfunctional

groups. These functional groups play an important role in the interaction with sorbed substances.

The sorption of  $Ag^{+}$  ions into reconstituted fibroin material from a solution of silk fibroin is well studied. The sorption capacity of  $Ag^{+}$  ions to the prepared sorbent has been found to be 62.5 mg/g [9]. It is recommended to separate silver ions from wastewater using this type of sorbent. Selective sorption of  $Cd^{2+}$  ions on a membrane-based on silk fibroin has been studied [10]. In addition, the sorption of many heavy metal ions and the effects of sorbed ions on the fibroin molecule have been identified [11].

In addition, many quantum chemical calculations have been performed to determine the effect of different media on the structure of silk fibroin [12]. The effect of water on the structure of silk fibroin and the change of crystalline particles have been studied using quantum chemical calculations [13].

In previous editions, we have provided information on how to obtain powdered "HF" [14]. In our study, we studied the sorption of silver, gold, and copper ions into powdered "HF" and changes in post-sorption processes using Charmm22 force field calculations.

\* Corresponding author.; e-mail: olmos77@mail.ru