Title: Insights into the preparation of Bi₂S_{3(core)}@SiO_{2(shell)} nanoparticles Student: David Doblas Moreno Date: January 2020 Supervisor/s: Dr. Juan C. Paniagua Departament de Química Física Dr. Carlos Moya Álvarez Departament de Física de la Matèria Condensada Dr. Xavier Batlle Gelabert Departament de Física de la Matèria Condensada

Computed tomography (CT) is an X-ray based whole body imaging technique widely used to enhance the contrast among human body tissues. Currently clinically CT contrast agents most used in humans are iodinated molecules or barium suspensions, but they have short circulation time and large doses are needed to provide good contrast. Nanoparticles (NPs) show potentiality for cell-tracking and higher residence times compared to these small molecules due to their functionalizable surface. Particularly, bismuth sulfide (Bi₂S₃) NPs are interesting because bismuth shows a large X-ray attenuation coefficient that enhances the contrast for small variations of the X-ray voltage. In addition, it is cheaper and exhibits lower toxicity than other metals with similar X-ray attenuation coefficients. The choice of a synthesis method is also of key importance to obtain Bi₂S₃ NPs with a good control over their structural properties.

Within this framework, we show the preparation of Bi₂S₃ NPs by the reaction of bismuth (III) neodecanoate (Bi(neo)₃) with thioacetamide in 1-octadecene by the hot injection method. We have monitored the particle size and shape by tuning both reaction temperature and time of the last step. Then, we have used the microemulsion method to encapsulate with silica a selected sample of Bi₂S₃ NPs in order to provide a hydrophilic surface for making Bi₂S₃ NPs suitable for in vitro CT experiments. Finally, these systems may pave the way to enable the combination with other materials to achieve multifunctional systems for diagnosis or theranostics.

Keywords: Bismuth sulfide nanoparticles, colloidal chemistry, silica encapsulation, X-Ray computed tomography.