

Spectroscopic and theoretical investigation insights into Stable Nano-HUP mediated by Bacteria

Xiaoqin Nie^{1,3}, Faqin Dong², Mingxue Liu², Edward O'Loughlin³, Maxim I. Boyanov³, Kenneth M. Kemner³

¹Fundamental Science on Nuclear Wastes and Environmental Safety Laboratory, Southwest University of Science and Technology, Mianyang 621010, PR China, xiaoqin_nie@163.com

²Key Laboratory of Solid Waste Treatment and Resource Recycle of Ministry of Education, Southwest University of Science and Technology, Mianyang 621010, PR China

³Bioscience Division, Argonne National Laboratory, Lemont, IL 60439, USA

In this study, *Kocuria rosea* (G+) and *Shewanella putrefaciens* (G-), isolated from an uranium mine area, has been chosen as model bacteria. By using of mesoscopic and advanced means of spectroscopy combined the simulated calculation, we identified the occurrence form and microstructure of uranium in and on the bacterial cells at molecular level. The sorption of U(VI) mediates the occurrence of uranium biominerals. U(VI)-phosphate mineral significantly formed after 24 hours contact with U(VI). The hydrogen uranyl phosphate(HUP) became the main products on the living *Kocuria rosea* and *Shewanella putrefaciens* with prolonged reacting time by EXAFS and XRD analysis. Uranium phosphate biomineralization was the prevalent U(VI) immobilization mechanism for living *Shewanella putrefaciens* without EPS at slightly acidic environments. HUP cannot formation when the the cytoplasm of bacterial was extracted. The adsorption energy was between -109kcal/mol and -114kcal/mol. The adsorption was easy to be spontaneous, and the energy was dominated by relaxation deformation adsorption energy. In the presence of carbonate, the probability of uranyl binding to biological phosphorus macromolecules will be restricted to some extent. The phosphate groups have a strong affinity to uranium atoms in uranyl, and the driving force of uranyl ions binding to phosphorus containing macromolecules in the wall membrane is mainly related to electrostatic force and van der Waals force.