





PROJECT TITLE: Design, synthesis and implementation of sustainable materials for heavy metal remediation in rivers

DTP Research Theme(s): Changing Planet

Lead Institution: University of Bristol

Lead Supervisor: Prof. Neil Allan, UoBristol, Chemistry **Co-Supervisor:** Prof. Steve Parker, UoBath, Chemistry

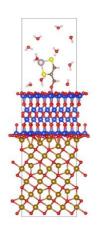
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Project keywords: metal remediation, nanoparticle synthesis and characterization, simulation,

biomolecules, inorganic geochemistry





Illegal gold mine in Colombia

Simulation of capturing mercury on a functionalised nanoparticle

Project Background

Colombia is a country with many natural resources including strategic minerals such as tungsten and gold. But low-tech and artisanal mining is not only destroying the large number of tropical forest in many regions of the country, but a particularly serious consequence is water contamination by direct dumping of mercury compounds used to isolate the gold. Mercury attacks the central nervous system, affects brain functioning and eventually leads to death; mercury pollution poses a major threat to human health in many developing countries, including South America and especially in Colombia. A 2017 BBC documentary highlighted that there are 17,000 illegal gold mines in the country, 80% of gold production is illegal and more profitable than drug trafficking. This is the source of most mercury pollution worldwide and per capita Colombia is the biggest mercury polluter in the world.

Project Aims and Methods

The overall project aim is to design, fabricate and implement in the field, new composite materials for the capture and subsequent removal of recognised heavy metal pollutants in contaminated water, predicted and characterised using state-of-the art atomistic simulation and experimental techniques.. The approach involves computational studies to identify molecules and materials with appropriate binding affinities in locally abundant natural resources. These species are then chemically engineered to enhance their activity by for example increasing the surface area or incorporating magnetic materials to allow ease of separation. As outlined above the initial environmental focus is the specific issue of mercury pollution in Colombia where in pilot studies "bottom up" modelling and atomistic simulation techniques have been used to explore the mechanisms of adsorption of a range of possible candidate biothiols (extracted from abundant local foodstuffs) at different silica interfaces. This provides a clear starting point for experimental optimisation of a nanostructured composite for mercury removal from contaminated waters in conjunction with further modelling to establish relationships between surface structure and affinity for mercury. There is flexibility to focus on computational and experimental aspects of this system or to identify new targets and interfacial chemistries, depending on the project direction desired by the student.



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Candidate Requirements

A background in physical or earth sciences with preferably undergraduate project experience in one of the key areas of materials synthesis/characterization/computation. We welcome and encourage student applications from under-represented groups. We value a diverse research environment.

Partner

A key goal of this project is to develop interfacial chemistry that allows effective uptake of polluting species onto recyclable surfaces. The strong computational component enabled by the expertise of Professor Steve Parker (Bath) in both interface and contaminant modelling reflects the importance of developing in silico model systems for testing in the lab.

Training

The student would receive training in all aspects of the project, in state-of-the-art experimental and computational methods. Training will also be provided in materials synthesis (nanoparticles, porous materials) and characterization techniques (BET, TEM, SEM). The initial target system is mercury and we have already established strong links with Colombia where opportunities already exist. There will be the opportunity to visit the Colombian research group at the Universidad del Norte, Barranquilla, Colombia, headed by Professor Carlos Pinilla and this will include visits to local industries there (Aquaterra Engineers SAS, developing and implementing solutions for problems in environmental and coastal engineering and (ii) LMB Laboratorios S.A.S, who specialise in water analysis and are keen to collaborate. We also have technical support there from the Alexander von Humboldt Institute for Natural Resources. The student will also be able to help identify other suitable systems for remediation and help develop networks in relevant countries as required.

References / Background reading list

Yu J.-G. et al, 2016, Environ. Sci. Pollut. Res. 23, 5056

Useful links

http://www.bristol.ac.uk/chemistry/courses/postgraduate/

Bristol NERC GW4+ DTP Prospectus:

http://www.bristol.ac.uk/study/postgraduate/2023/doctoral/phd-great-western-four-dtp/

How to apply to the University of Bristol:

http://www.bristol.ac.uk/study/postgraduate/apply/

<u>Please note:</u> If you wish to apply for more than one project please contact the Bristol NERC GW4+ DTP Administrator to find out the process for doing this.

The application deadline is Monday 9 January 2023 at 2359 GMT. Interviews will take place during the period 22 February – 8 March 2023.

NERC GW4+ DTP Website:

For more information about the NERC GW4+ Doctoral Training Partnership please visit https://www.nercgw4plus.ac.uk.

General Enquiries:

Bristol NERC GW4+ DTP Administrator Email: bristol-nercgw4plusdtp-admin@bristol.ac.uk

