**Project Title:** "Hard" metals: Looking for alternative material for high temperature applications

**Supervisor(s):** Dr Lorenzo Stella and Prof. Robert Bowman

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**Type of Project:** Computational/Theoretical

**Helpful existing knowledge:** A basic knowledge of quantum mechanics and solid-state physics would be useful, but not essential.

**Funding status:** Unfunded yet, but funding may become available at a later stage for UK and RoI residents.

## Project Description

Good metals like copper and gold deploy many electrons to conduct electricity, but are ductile (or "soft"), especially at high temperature. Ceramic materials are "hard" and heat-resistant but are bad electrical conductors. Can we find a "hard" metal or alloy with good conductivity that resists mechanical deformation at high temperature? Far from being an academic question, an affirmative answer will have tangible practical consequences, also for you! Given an ever-increasing demand for data storage, the technology behind hard disk drive (HDD) has been pushed to the limit. Heat-assisted memory recording (HAMR) use a metallic near-field transducer (NFT) to write on very small (a few nanometres!) magnetic domains, and then increase the HDD capacity. Due to its electrical and chemical properties, gold is the current material of choice, but there are mechanical drawbacks that limit its reliability for current HAMR technology. A "hard" metal or alloy with properties comparable to those of Gold, and yet not as "soft" as Gold, is wanted for this job.

In practice, the successful candidate will model the dielectric properties of material candidates, such intermetallic and heavily doped metal oxides, at high temperature using first principles approaches like *ab initio* molecular dynamics and (time-dependent) density functional theory. The project builds on the results of a previous PhD project (yet unpublished). Early results of this project will be compared against experimental findings obtained by the group of Prof. Robert Bowman and Dr Fumin Huang. At a later state, the successful candidate is expected to predict material properties that may inform the design of new experiments, and possibly suggest better performing "hard" metal candidates.

## Skills gained by the student

By completion of the project, the student is expected to have a good control of advanced numerical methods to model time-dependent response of complex materials. Those methods can include existing implementations in electronic structure code and custom code developed during the project. The student will have the possibility to train written and presentation skills by writing articles and presenting at conferences. Opportunities for additional training and development (*e.g.*, to prepare fellowship applications) will be provided by the QUB Graduate School.

## Useful references

- Plasmonic near-field transducer for heat-assisted magnetic recording
- Materials for heat-assisted magnetic recording heads
- A review of the optical properties of alloys and intermetallics for plasmonics
- Optical properties of Au-Hf thin films