# Computational Materials and Minerals Group

**Our Website:**
**cmm-group.github.io**

**Job Vacancies**

## Our Story

SCAN ME

We are the Computational Materials and Minerals Group, CMM Group, based in the Department of Chemistry at the University of Huddersfield.

We apply fundamental and exciting scientific research in materials science, solid state and computational chemistry.

The performance of materials and minerals lies at the heart of the development of green sustainable technologies, and computational methods play a vital role in modelling and predicting the structures, properties and reactivity of complex materials.

## PhD Studentships

EPSRC Engineering and Physical Sciences Research Council

Application Deadline: 28th February 2020
Start Date: 1st October 2020
All enquiry to **m.molinari@hud.ac.uk** and **d.j.cooke@hud.ac.uk**

SCAN ME **Molecular Simulation Studies of Candidate Enzymes and their Inhibitors for the Design of Anticancer Drugs**

SCAN ME **Multifunctional Enzyme Mimetic Oxide Nanomaterials for Therapeutic Technologies**

SCAN ME **Fluorite Materials for Solid Oxide Fuel Cell Technologies**

## Comments from Current PhD students

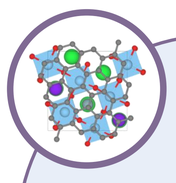
"I had the opportunity to gain **coding skills in Python, HTML, CSS, Fortran and LaTeX** without having any previous experience when started."

"Working in **materials science has opened new career opportunities** in academia as well as in R&D jobs in industry."

"**I like research** and I feel **this PhD has made me grow** both academically and personally."

"**I don't like experimental labs.** Now I work comfortably in an office with a laptop!"

## Our Research

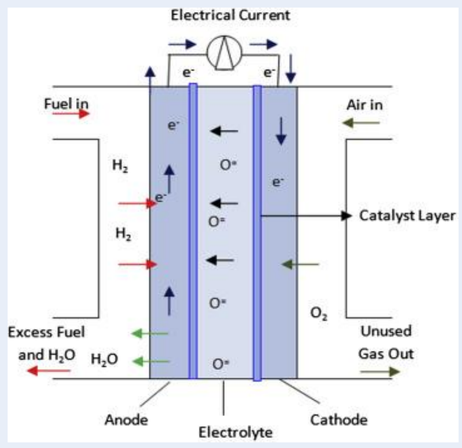


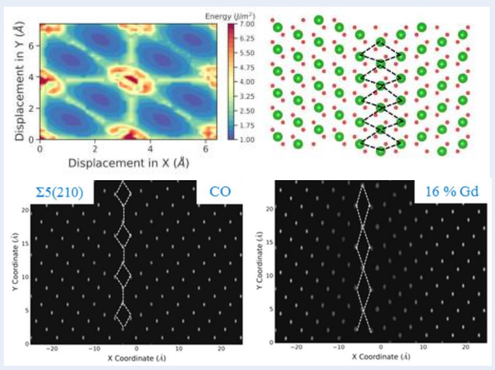
## Energy Materials

Energy provision is one of the most important challenges for society.
We study solid electrolytes for energy generation, storage and recovery.

**Solid Oxide Fuel Cell.** Fluorite structures, like doped $ZrO_2$ and $CeO_2$ are among the most promising solid electrolytes. This technology has low environmental impact but high running costs due to high operating temperatures required.

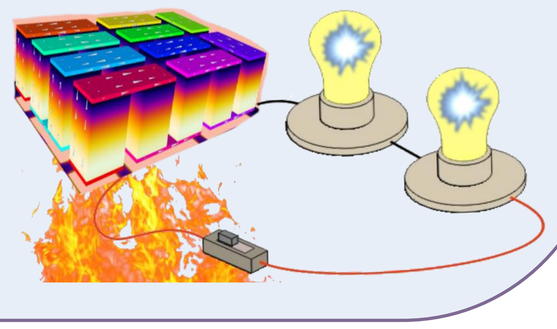
**Doping and nanostructuring are strategies to reduce operating temperatures.**



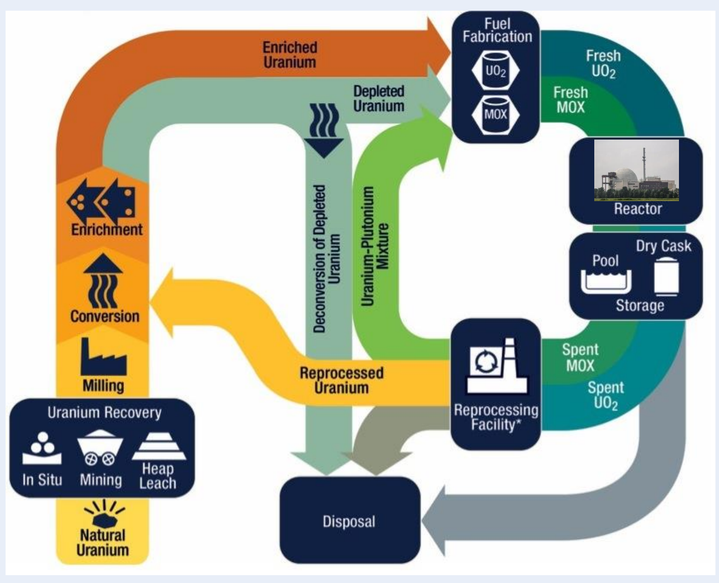




**Interfaces** can be introduces to enhance ion conductivity. However these interfaces may change structure upon **dopants segregation**.

**Thermoelectric devices.** Perovskites such as $SrTiO_3$ and its composites with graphene are promising materials for waste heat recovery, and efficiently convert waste heat into electricity.

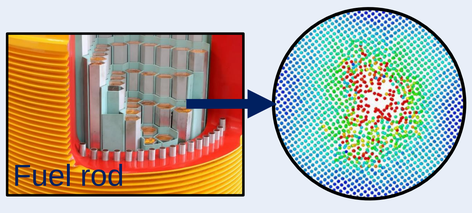


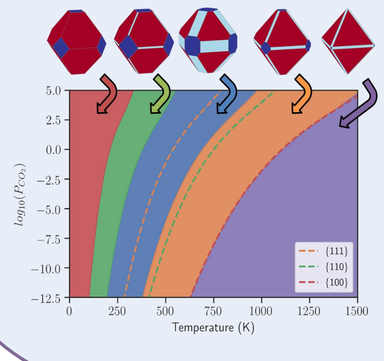
## Nuclear Materials




**Modellers study radiation processes on a timescale that is unattainable using experiments.**

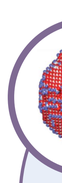
High performance computers can simulate the effects of high energy radiation on structural materials in a nuclear reactor.




**Storage and disposal of nuclear materials may have potential risks to human and the environment.**

Computational techniques can predict the long term behaviour of nuclear materials. For example we have predicted the morphology of $PuO_2$ nanoparticles in relevant conditions to storage and disposal of the materials.



## Materials for Medical Applications

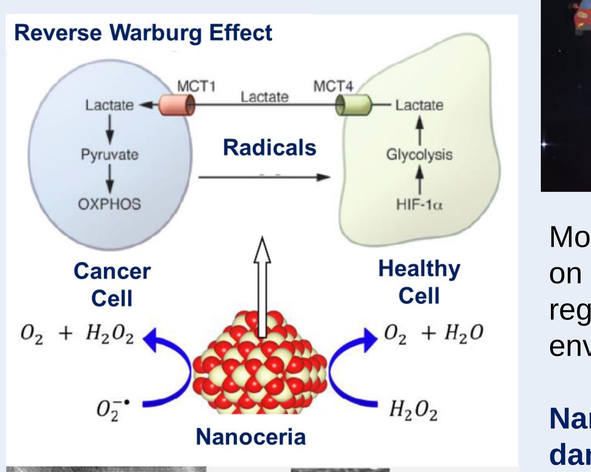
**Nanozymes** are nanoparticles with enzymatic mimetic activities, with lower cost, and higher stability and durability than natural enzymes.

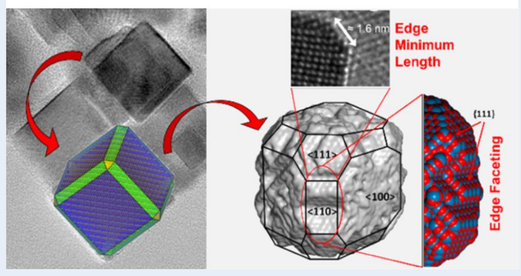
Nanozymes have potential usage as **new therapeutic agents for cancer, and degenerative diseases.**

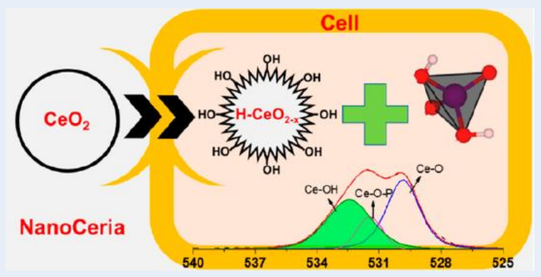

Modelling the reactivity of nanozymes based on **cerium oxide** will allow us to selectively regulate their activities within biological environments.

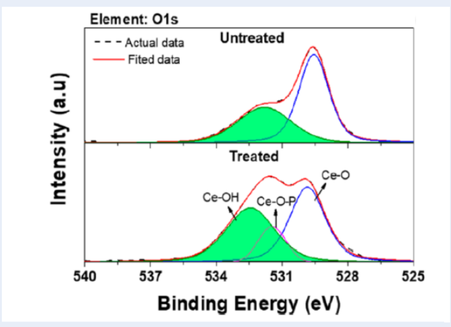
**Nanoceria can disrupt the production of dangerous reactive oxygen species and thus interfere with cancer growth.**

However, we need to be able to determine the response of nanozymes to biological media. Modelling can predict nanozyme morphologies that can resist to phosphate scavenging and thus retain their enzymatic activity.




**Organometallic complexes offer the prospect of targeting multiple pathways that are important in cancer biology.** A silver-bis(N-heterocyclic carbine), complex (Ag8) induces cancer cell death.

Lactate Dehydrogenase A (LDH-A) is the enzyme that catalyzes the conversion of pyruvate to lactate and thus is essential to cancer metabolism (Warburg effect). There is an ongoing effort to identify effective inhibitors that will not only block the function of the enzyme but will also have minimal side effects.