

## PhD Candidate Profile

**Name:**

Ciara Byrne

**Research Group:**

Nanotechnology Research Group

**Research Centre:**

The Centre for Precision Engineering, Materials & Manufacturing research (The PEM Centre)

**Department/School:**

Department of Environmental Science, School of Science

**College:**

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**Supervisor:**

Prof. Suresh Pillai

**Funding body:**

IT Sligo President's Bursary

**Area (field) of study:**

Titanium dioxide photocatalysis

**Thesis Title:**

Understanding the Mechanism of Anatase to Rutile Transition in Titania Photocatalysis

**Abstract:**

Titanium dioxide is one the most researched photocatalyst as it is nontoxic, the ease of preparation, its strong oxidising ability, availability and its long-term stability. Titanium dioxide (titania) has three main crystalline phases, anatase (tetragonal,  $a=b=3.78\text{\AA}$ ;  $c=9.50\text{\AA}$ ), brookite (rhombohedral,  $a=5.43\text{\AA}$ ;  $b=9.16\text{\AA}$ ;  $c=5.13\text{\AA}$ ) and rutile (tetragonal,  $a=b=4.58\text{\AA}$ ;  $c=2.95\text{\AA}$ ). Rutile has been reported as the most thermodynamically stable phase and is the phase most abundantly found in nature. Anatase and brookite are both metastable phases, they irreversibly transform into rutile at temperatures between 600-700°C in pure synthetic titanium dioxide. Of the three phases, anatase is considered to be the most photocatalytic active phase. Different chemical additives/dopants can be used to extend the anatase to rutile phase transition to higher temperatures. The ability to make high temperature ( $\geq 800^\circ\text{C}$ ) stable anatase phase with photocatalytic properties is required for some its applications.



The main objectives of this work are:

- The chemical synthesis (sol-gel and microwave assisted synthesis) of titanium dioxide nanomaterials with a number of different precursors (e.g. titanium isopropoxide or titanium butoxide).
- Calcining all samples at temperatures between 400-1100°C for the purpose of determining the temperature the anatase to rutile occurs at.
- To add a number of different chemical additives/dopants in varying concentration and examine how this affects the transition from anatase into rutile.
- To examine how the above factors affect the photocatalytic activity of titanium dioxide.
- To use titanium dioxide as a photocatalyst for environmental applications, e.g. for water treatment.
- The samples will be characterized by X-Ray Diffraction (XRD), Field Emission Scanning Electron Microscopy (FESEM), Transmission Electron Microscopy (TEM), X-ray Photoelectron Spectroscopy (XPS), Fourier Transform Infrared Spectroscopy (FTIR), Raman spectroscopy and gas phase photocatalysis studies.

### Collaborations:

- University of Surrey
- Dublin Institute of Technology

### Publications:

N/A

### Presentations:

The 25<sup>th</sup> Irish Environmental Researcher's Colloquium (ENVIRON) in Nanotechnology (April 2015)

