

## **Nanoscale moving boundary problems**

### **Group Leader:**

Tim Myers  
[tmyers@crm.cat](mailto:tmyers@crm.cat)

### Area(s) of Knowledge:

- Physical Sciences, Mathematics and Engineering

### Group of disciplines:

PHYSICAL SCIENCES, MATHEMATICS AND ENGINEERING

Theoretical and Applied Mathematics,  
Materials,  
Nanotechnology

### Research project/Research group description (màx. 2.000 caràcters)

Lying at the heart of nanotechnology is the nanoparticle, a unit of matter with at least one length-scale between 1 and 100 nm. Nanoparticles are increasingly employed in electronics, energy production and storage, medicine and materials. It is estimated that the market for semiconductor nanocrystals alone will have a value of over \$4 billion by 2020.

The properties of nanoparticles are size dependent and consequently often exhibit unexpected behaviour, so leading to new forms of mathematical model. The proposed project will deal with two mathematically related topics: the growth of nanocrystals in solution and their response to harsh thermal environments. In both cases the basic model involves a form of diffusion equation applied over an unknown, moving boundary.

### Nanocrystal growth

Since nanocrystal properties depend on their size it is essential to be able to produce particles of a specific size in a controlled manner. This requires a clear understanding of the growth process. Currently the most common production method is from a colloidal solution. Recently members of the Industrial Maths Research Group (IMRG) demonstrated that the standard theoretical model, used to describe the growth of a single crystal and employed for over 100 years, is not applicable to the majority of nanocrystal growth processes. The aim of this project component is to advance the new model and then apply it to a system of particles, with the ultimate aim of guiding future large scale production processes.

### Nanoscale phase change

In many applications, such as drug delivery, phase change memory and nanolithography, nanoparticles are subject to high temperatures. It is well-known that the classical description of heat flow, based on Fourier's law, breaks down at small length and time-scales. The IMRG has been working in collaboration with physicists on developing and analysing novel models to describe nanoscale heat flow. The current challenge is to adapt these models to phase change, particularly melting, of nanoparticles.