



# Invitation to the Parker Centre Science Conversation 7

**The Parker Centre invites you to the seventh session  
in its Science Conversations seminar series**

- Topic:**           **Biomolecular Controls on Mineralisation**
- Presenter:**   **Professor Jim de Yoreo**  
Lawrence Berkeley National Laboratory, California, USA
- Date:**            Wednesday 7 May 2008
- Venue:**          New Seminar Room, Australian Minerals Research Centre  
(AMRC), Conlon St, Waterford  
(Enter into the AMRC car park from Conlon St (off Manning Rd),  
New Seminar Room is next to the reception desk)
- Time:**           4.00–5.00pm; presentation followed by light refreshments

**Abstract:**

The complex shapes and hierarchical designs of biomineral structures arise from biomolecular controls over crystallisation. This process of biomineralisation plays a key role in both environmental geochemistry and human health and medicine. Moreover, it has become a source of inspiration to materials scientists seeking novel routes towards synthesis of new materials. One prevailing view of the process is that mineral-associated macromolecules are responsible for nucleating and stabilising non-equilibrium polymorphs and morphologies through interactions at crystal surfaces. But a quantitative understanding of molecular interactions between modifiers and crystal surfaces and the changes in growth mechanism induced by those interactions has been lacking.

In order to develop that understanding, we are combining *in situ* AFM with molecular modeling methods to explore the effect of peptides and proteins on the growth of calcium carbonates, phosphates, and oxalates. We are also using NEXAFS and *in situ* TEM to investigate the process of templated nucleation of carbonates on self-assembled monolayers (SAMs) with amino acid functionalities.

In this talk, I will first present common themes that have emerged from AFM studies of the effects of aspartic acid-rich peptides and proteins on the growth of calcite and calcium oxalate monohydrate (COM). The results show how the interactions between the biomolecules and the molecular features on crystal surfaces lead to changes in growth morphology and kinetics. Those changes are then linked to the underlying stereochemical relationships and energetic controls using molecular modeling techniques. Then, by



## Parker Centre

analysing the AFM results using classical crystal growth theories combined with kinetic Monte Carlo simulations, the physical mechanisms that lead to growth modification are identified.

In the second part of the talk, I will present the results of the NEXAFS investigations, which show that the pathway to directed formation of calcite on SAMs passes through an amorphous calcium carbonate phase, whose appearance is accompanied by a loss of SAM order. Transformation of this phase to oriented calcite eventually takes place via a dissolution-precipitation reaction, but from SEM studies it appears that this transformation advances through the amorphous material by starting at the film-mineral interface. Analysis of nucleation rates on various SAMs suggests that small reductions in interfacial energy drive this process.