# Condensed Matter Physics Institute Seminar

## 13:00 | Tuesday 20th September | G/020

# Computational Chemistry Downunder: from Ice Inhibition to Minerals

Prof. Paulo Raiteri

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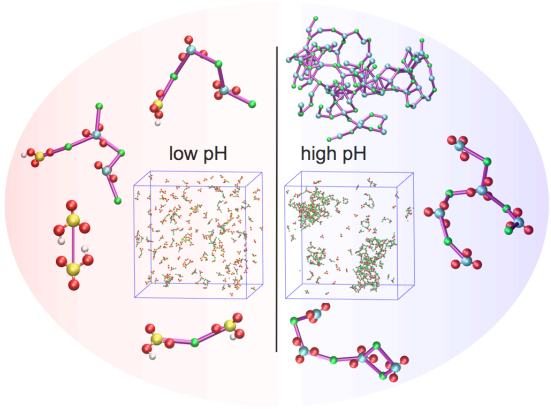


Crystal growth is ubiquitous in many fields from pharmacology to engineering, and being able to predict which crystals form under a given set of environmental conditions would produce enormous benefits to many applications, such as drug delivery, scale inhibition and cryopreservation, to name a few. In this presentation, I will show the recent advances towards understanding crystallisation made in in the computational chemistry group at Curtin University. In particular, I will focus on the problem of calcium carbonate growth and discuss the existence of stable pre-nucleation clusters. Since their existence was proposed by Gebauer and Cölfen in 2008[1] they have proven to be elusive because their extreme small size and dynamics place them in a "*dark area*" where both experimental techniques and computational methods struggle to give accurate and reliable answers. I will also discuss the accuracy and limitations of current computational techniques and suggest possible ways forward to better understand nucleation and growth in complex systems.

Short Biography:

Paolo Raiteri obtained is MSc and PhD in Materials Science from the University of Milano-Bicocca in 1999 and 2003, respectively. He then moved to the ETH Zurich to undertake a post-doc under the mentorship of Prof Parrinello. In 2008 Paolo Raiteri moved to Australia as an early Career Research Fellow at Curtin University. In 2009 and 2013 he was awarded two fellowships from the Australian Research Council (ARF and Future Fellowship). In 2014 he became a tenured staff member in the Department of Chemistry at Curtin University and in 2015 was promoted to Associate Professor. So far Paolo Raiteri has published 66 papers, has received more than 2300 citations in peer reviewed journals and has an h-index of 25.

[1] Gebauer, D.; Voelkel, A.; Coelfen, H. Stable Prenucleation Calcium Carbonate Clusters. *Science* **2008**, *322*, 1819–1822.