CNMS DISCOVERY SEMINAR SERIES

Thursday, March 1, 2012
4:00 pm
Iran Thomas Auditorium, 8600

Simulating the Formation of Carbonate Minerals: The Role of Nanoscale Phenomena in Non-Classical Nucleation

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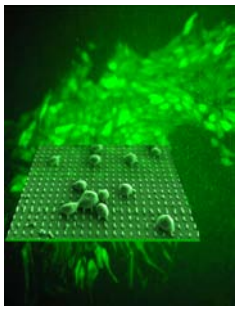
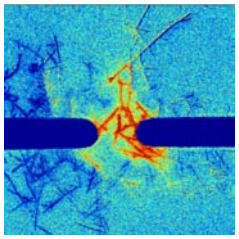
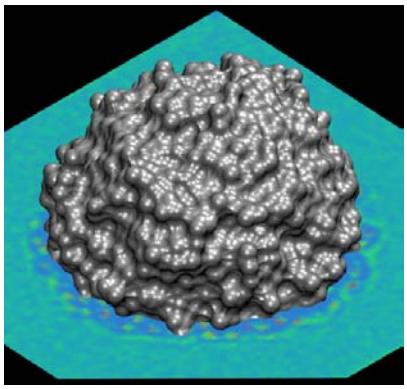




Abstract:
Calcium carbonate is an abundant mineral that exhibits three crystalline polymorphs, as well as an amorphous form, and represents a natural form of sequestered carbon. While the most stable calcite polymorph can grow as macroscopic single crystals, the process of biomineralisation can alternatively lead to complex polycrystalline assembles that serve as functional materials in nature. As such, the biomineralisation of minerals represents the ultimate in crystal engineering and the challenge is to understand these processes at the atomic level. Currently, even the simple homogeneous nucleation of calcium carbonate remains to be fully comprehended. Recent experiments have demonstrated this process may go against classical theories of nucleation [1,2], though how and why this happens is unclear.



In this presentation the combined use of computer simulation and experiment will be explored to try to unravel the complexities of the growth processes for calcium carbonate. Through understanding the thermodynamics of crystalline versus amorphous nanoparticles [3], as well as the nature of stable pre-nucleation clusters and interfacial properties [4], a model is found to emerge in which the different behaviour of materials at the nanoscale can explain the non-classical formation of calcium carbonate.

References:
[1] D. Gebauer *et al*., *Angew. Chem. Int. Ed.*, **49**, 8889 (2010)
[2] D. Gebauer, A. Völkel and H. Cölfen, *Science*, **322**, 1819 (2008)
[3] P. Raiteri and J.D. Gale, *J. Am. Chem. Soc.*, **132**, 17623 (2010)
[4] R. Demichelis, P. Raiteri, J.D. Gale, D. Quigley and D. Gebauer, *Nature Comm.* (in press)

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