

GEMSEC SEMINAR

GENETICALLY ENGINEERED MATERIALS SCIENCE AND
ENGINEERING CENTER, AN NSF-MRSEC AT THE UW

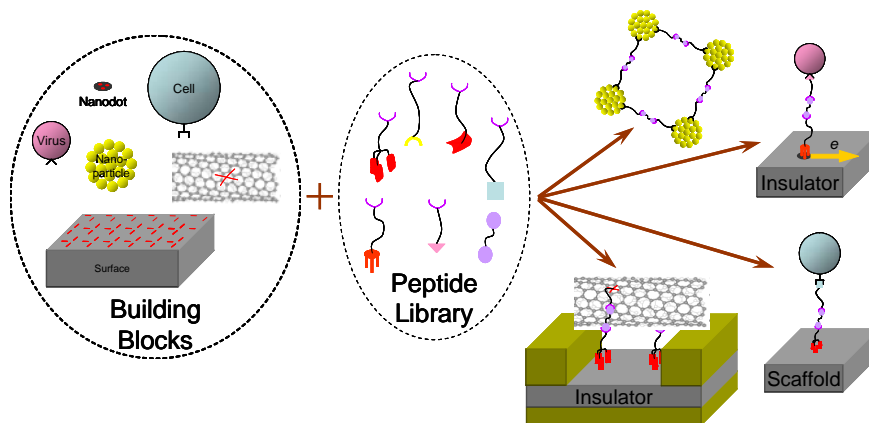
Thursday, February 14, 2008, 1:30 pm
Milnor Roberts Room, 243 Wilcox
Materials Science and Engineering

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Towards Rational de novo Design of Peptides for Inorganic Interfaces

Proteins at inorganic interfaces occur across science, technology and nature – protein arrays, prostheses such as stents and artificial heart valves, biomimetic assembly of nanoparticles, and anti-freeze proteins are just a few examples from many. Despite the clear importance of proteins at inorganic interfaces, elucidation of the structure and behavior of proteins at such interfaces and the design of associated systems is still dominated by experiment, and trial and error. We at Edinburgh are developing computational tools that will complement this experimental effort.



Peptide-mediated self-assembly is thought (Mirkin & Taton, *Nature* **2000** 405, 626) to be one of the best routes to the 'holy grail' (Ball, *Tech. Rev.* **2001**, 104, 31) of mass production of nanostructures and materials (top) and nanoelectronics (bottom), whilst surface-binding peptides are underpinning new biosensor (c-top) and tissue engineering (c-bottom) technologies.

In this seminar, I will outline the overall approach we are seeking to develop for the rational *de novo* design of systems involving proteins at solid interfaces – which exploits *in silico* evolutionary processes – and then provide details (with examples) of the various elements involved.

As part of this, I will present results for the *ab initio* prediction of protein conformations in the gas and liquid phases and at solid surfaces, and a molecular switching phenomenon we have observed in polyalanine that may be of relevance to nanotechnology and disease processes.

**Dr. Biggs is a Senior Lecturer in Chemical Engineering Science and Royal Academy of Engineering/Leverhulme Senior Research Fellow at the University of Edinburgh in Scotland, United Kingdom. His research is focused on the modelling of interfacial systems for the elucidation of fundamentals and design.*