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The Chinese University of Hong Kong
Department of Chemistry
Research Seminar Series

Speaker: Professor Alex Edwin Bunker
Faculty of Pharmacy
University of Helsinki

Title: Computationally assisted design (CAD) for drug delivery; Molecular dynamics modelling as a tool in nanomedicine: Liposome based drug delivery systems as a case study

<< *Abstract* >>

The development of nanoscale drug delivery mechanisms, nanomedicine, is one of the most promising new avenues for drug delivery. It carries the promise of extending the solubility profile of drugs that can be delivered, and effectively targeting the delivery to the desired tissue, thus increasing efficacy and reducing side effects. This field has so far, however, been far better at generating new publications than new approved drug therapies. Part of the cause of this is the extent to which trial and error based methodologies continue to dominate the drug development process. While several experimental techniques exist to investigate aspects of the behavior of nanoscale drug delivery mechanisms, there remain considerable gaps of knowledge. Computational molecular dynamics modelling (MD) with a model with all atom resolution has the potential to integrate these results, and allow for a rational design approach to be applied: engineering devices instead of trial and error development of drugs. We have performed a considerable amount of work using MD to gain insight into the structure and behavior of liposome based drug delivery systems (LDS). This can be seen as a case study of the potential for computational modeling to be used, alongside complementary experiments, to achieve a design based approach in nanomedicine.

Date: January 13, 2017 (Friday)

Time: 4:30 p.m.

Venue: L1, Science Centre

ALL ARE WELCOME

Contact Person:
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