



## ***A Short Introduction to the Reverse Monte Carlo Technique - Theory, Application and Software***

by Mr Andreas Hall

**Date: 14<sup>th</sup> May 2009 (Thursday)**

**Time: 12:00pm to 1:00pm**

**Venue: EA-02-11 (Executive Seminar Room)**

### **Abstract**

A reoccurring problem in the investigation of amorphous materials and crystalline materials with partial disorder is the creation of realistic, atomic-scale structure models in order to fully understand e.g. atomic diffusion, phase transitions, etc. The reverse Monte Carlo method (RMC) uses a variation of the Metropolis Monte Carlo (MMC) algorithm where the agreement between calculated properties of the model and experimental data is used as the driving force, rather than a minimization of the total energy of the model. While RMC rids us of the problem of finding sufficiently good inter-atomic potentials, it requires more experimental knowledge of the system in order for it to produce a physically sound model structure.

The presentation gives a brief overview of the RMC technique, with some focus on its application to amorphous systems. Discussion will cover underlying theory, overview of its uses, modeling in practice and a glance at currently available software.

**Mr Andreas Hall    Speaker**

In December 2008, Andreas Hall presented his PhD thesis, *Ionic Conduction and the Bond Valence Method in Glasses*, containing his work on the atomic structure and ionic transport pathways in borate and phosphate glass systems, performed at the Chalmers University of Technology, Gothenburg / Sweden. He is currently employed as a research fellow by Dr. Stefan Adams at the Material Science and Engineering department at NUS.

**Dr Xue Jun Min Host**

*All are Welcome!*