NITheP cordially invites you to a seminar by:

Prof. Alex Welte
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Date:       Wednesday 24th of November 2010
Time:       15:00
Venue:      NITheP Stellenbosch Seminar room

**Title:** The Correlation Problem for Electrons in Molecules: A Systematic Scheme of Corrections beyond a non trivial Self Consistent Field Approximation

**Abstract:** The electronic structure of molecules depends in detail on a precise handling of electron-electron correlation, but the number of 'many electron' degrees of freedom proliferate unmanageably according to combinatorial factors arising from the number of single electron degrees of freedom introduced in the discretisation of the kinetic energy through a cut-off of some kind. Electronic structure calculations typically use a non interacting electron gas, or a pseudo non interacting electron gas (Hartree Fock) as a zero order approximation on which to build either perturbation theories of truncated spaces defined by the number of (or independently optimised number of) 'particle-hole pairs'. This usually leads to the need for high order corrections, which are computationally impractical for many large interesting problems, such as molecules involved in biological processes. In this talk we review the problem and present a variation on the traditional approach.

The new method uses Goddards 'Perfect Pairing Generalized Valence Bond' model as the zero order approximation. This offers a unique trade-off of computational cost against dynamical content. Both short and long term prospects for progress in this area are highlighted.

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