

AVVISO DI SEMINARIO

Mercoledì 30 gennaio 2008 ore 11.15

Aula A1 (III piano), Edificio C11, via Giorgieri 1, Università di Trieste

il dottor **Andrew M. Teale** del Centre for Theoretical and Computational Chemistry, Department of Chemistry, Oslo University (Norvegia) terrà un seminario su

Optimized Effective Potentials and Constrained Search Procedures in DFT

Abstract :

The implementation of the Optimized Effective potential method in Dalton is briefly outlined before discussing its application to Hybrid DFT functionals. The possible advantages of orbital dependent functionals over conventional density functionals are discussed and results for the calculation of NMR shielding constants are presented.

The closely related constrained search procedure will also be briefly outlined and results for NMR shielding constants presented. A generalization of this scheme to arbitrary density functionals will be presented as a way to calculate accurate adiabatic connection curves utilizing coupled cluster calculations.

Il Direttore
Prof. Lucio Randaccio

Tutti gli interessati sono invitati a partecipare