ΣΕΜΙΝΑΡΙΟ

ΟΜΙΛΗΤΗΣ: **Neil L. Allan**
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ΘΕΜΑ: **THINK LOCALLY (BUT ACT GLOBALLY!).**

ΤΟΠΟΣ: Αίθουσα Σεμιναρίων ΙΤΕ/ΕΙΧΗΜΥΘ

ΗΜΕΡΟΜΗΝΙΑ: **Τετάρτη, 14 Απριλίου 2010**

ΩΡΑ: **12:00**

ΠΕΡΙΛΗΨΗ:

We highlight the crucial influence of the local environment of individual cations on the structure and energetics of non-stoichiometric compounds, solid solutions and nanostructures, and discuss some new computational techniques we are developing to examine this. Consideration of average structures is NOT sufficient.

We consider a range of examples: (i) superionic conductors such as $Ba_2In_2O_5$, CuI and Bi_2O_3. (ii) the pyrope-grossular garnet solid solution where surprisingly long range interactions are important (iii) Thin films of mixed oxides. We emphasise the different insights gained into the solid state chemistry of these systems and the consequences for thermodynamic and transport properties.