ΙΤΕ/ΕΙΧΗΜΥΘ

ΣΕΜΙΝΑΡΙΟ

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ΘΕΜΑ: **Designing Nanoporous Materials for Hydrogen Storage**
Σχεδιασμός Νανοπορωδών Υλικών για Αποθήκευση Υδρογόνου

ΤΟΠΟΣ: Αίθουσα Σεμιναρίων ΙΤΕ/ΕΙΧΗΜΥΘ

ΗΜΕΡΟΜΗΝΙΑ: **Πέμπτη, 19 Ιουνίου 2008**

ΩΡΑ: **17:00**

ΠΕΡΙΛΗΨΗ: A combination of ab-initio and Monte Carlo techniques is used for investigating the nature of hydrogen interaction with different types of Nanotubes (C-NT, BN-NT, SiC-NT), Nanoscrolls (Fig.1) and Metal Organic Frameworks (MOFs Fig.2). In addition the improvement of the storage capacity is tested under various conditions of pressure and temperature after substitution and doping.

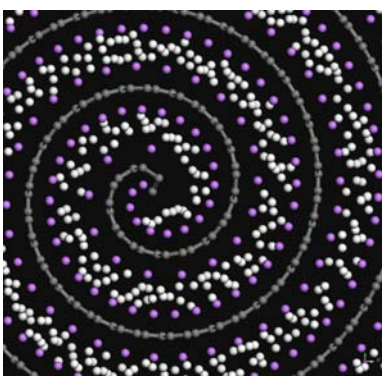

Figure 1: Model of Li-doped Carbon NanoScroll at T = 293 K and P = 100 Bar.

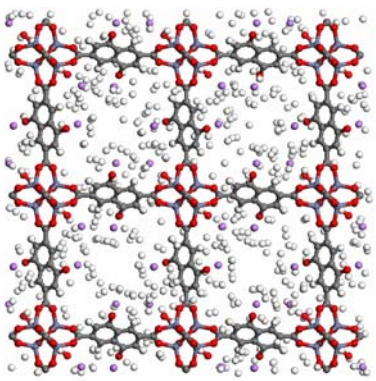

Figure 2: Model of Li-alkoxide modified IRMOF-8 at T = 77 K and P = 1 Bar.

ΣΕΜΙΝΑΡΙΟ

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