

Seminar Notice

*International Year of Chemistry - 2011 Seminar Series -
06*

Department of Chemistry
Pondicherry University, Puducherry – 605 014

Title

CARBON CHAINS AND METALS IN MOLECULAR WIRES. SYNERGETIC ELECTRONIC EFFECTS

By

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Date: 14th (Wednesday) December 2011

Time: 3.30 pm

Venue: Seminar hall, Department of Chemistry, PU

Head of the Department

Seminar Convener

CARBON CHAINS AND METALS IN MOLECULAR WIRES. SYNERGETIC ELECTRONIC EFFECTS

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ABSTRACT: In recent years, molecular compounds in which different carbon-containing units span two redox transition metal groups have received considerable attention, due to the speculation that such assemblies would be well suited for use in a variety of applications, including, for example, information storage devices. The control and manipulation of the interactions between the metal termini of such systems are therefore of great practical importance, but present considerable conceptual challenges. These challenges can be met by combining experimental studies with theoretical methods. We have ourselves analysed and compared the electronic and geometrical structures of a large variety of transition-metal systems containing different all-carbon spacers with the aid of density functional theory tools. More recently, incorporation of hetero-elements such as nitrogen or boron in the carbon spacers has been theoretically studied in order to consider their effects on the electronic interaction between the metal centres. Some recent results will be discussed.