## 2013 2

## Molecular wires: from metal-metal bonds to electron transport.

3 14

15: 00 - 16: 40 212

Abstract Molecules containing chains of metal ions linked by direct covalent metal-metal bonds bear a striking resemblance to macroscopidli wires, but just how real is this analogy? In this talk I will use a family of Extended metal Atom Chains (EMACs) to explore the relationship between structure, bonding and electron transport in metallic nanowires. In most cases the σ bonding framework dominates both the M-M bond strength and its ability to conduct electrons.

John McGrady is Professor of Computational Inorganic Chemistry at the University of Oxford, UK. His research interests centre on the application of density functional theory to problems of structure, magnetism and reactivity of

system<mark>s co</mark>ntaining

transition metal elements

Prof. John McGrady,

jinglu@pku.edu.cn