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

Prof. John McGrady

时间: 3月14日 (星期四) 15:00—16:40

地点: 北京大学物理大楼中212教室

Abstract: Molecules containing chains of metal ions linked by direct covalent metal-metal bonds bear a striking resemblance to macroscopic 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.

Prof. John McGrady, 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 systems containing transition metal elements.

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