

## CBC SEMINAR ANNOUNCEMENT



**Professor Karine Costuas  
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### **Functional Carbon-Rich Organometallic Compounds: Theoretical Aspects**

Molecular materials based on the assemblage of organometallic fragments and conjugated organic ligands are among the most studied compounds in coordination chemistry. This is due to their relatively good stability combined with their excited-state and redox properties which confer them interesting physical properties in several domains (magnetism, optics, electrochemistry...). These multifunctional systems are promising candidates to be incorporated in nanoscale devices for molecular electronics and/or spintronics.

The control and manipulation of the interactions between the metal termini of such systems are of great practical importance, but present considerable conceptual challenges. These challenges can be met by combining experimental and theoretical studies. Using results obtained from theoretical calculations of density-functional theory (DFT) type, some physical properties of representative compounds will be discussed. Particular emphasis will be put on the electronic reasons of the changes in structural and physical properties upon oxidation or reduction, or upon structure modification of metallic moieties and of the conjugated ligands.

<b>Date:</b>	<b>30<sup>th</sup> March 2012 (Friday)</b>
<b>Time:</b>	<b>3pm – 4pm</b>
<b>Venue:</b>	<b>NTU SPMS CBC Building Level 2, Conference Room</b>
<b>Host:</b>	<b>Assoc Professor Chen Hongyu</b>