Theoretical and Physical Chemistry Institute

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ONLINE LECTURE

"Copper Oxide (Cu_2O) and Copper Nitride (Cu_3N): Growth, Properties and Prospects for Energy Conversion and Storage"

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Abstract

Cu_3N is an earth abundant, indirect energy bandgap semiconductor, in which crystal imperfections such as N vacancies (V_N) and Cu interstitials (Cu_i), do not give rise to mid-gap states, but instead electronic states that are energetically located very close or inside the conduction and valence band edges respectively. Consequently, it has been proposed to be used as a defect tolerant semiconductor for energy conversion and the fabrication of solar cells, considering that bipolar doping is possible too. Besides, it has an anti-ReO_3 cubic crystal structure which makes it suitable for energy storage and the realization of batteries, so it is still an active topic of investigation.

In this talk I will describe the growth and fundamental properties of Cu_3N which is necessary to understand its potential for energy conversion and storage. We have observed the M and R direct energy band gaps of Cu_3N by ultra-fast pump-probe spectroscopy (UPPS), confirming that it has a 'clean' energy bandgap with no mid gap states in excellent agreement with density function theory calculations of the electronic band structure [1]. However, while Cu_3N exhibits 'clean' band gaps it has limited carrier lifetimes attributed to indirect, non-radiative, recombination via electronic states located very close to or inside the conduction and valence bands. Consequently, the original suggestions that it may be used as a defect tolerant semiconductor need to be interpreted accordingly. Furthermore, I will describe ongoing work and the current challenges in the growth of high quality Cu_2O which has been proposed for a long time to be suitable as a solar cell absorber but also recently for the purpose of catalysis and carbon dioxide reduction.

[1] M.Zervos, A.Othonos, M.Sergides, T.Pavloudis and J.Kioseoglou, Observation of the Direct Energy Bandgaps of Defect Tolerant Cu_3N by Ultrafast Pump Probe Spectroscopy, *J.Phys.Chem.* C (2020).