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DFT+U Study of CuO Surfaces and Vacancy Formation for CuO Nanowires-CNTs Hybrid Electrode in Supercapacitors

Supercapacitors are attracting considerable interest for clean energy storage applications due to their high specific capacitance, fast charging-discharging, long cycle life and non-toxicity. Many attempts have been made to increase performance of electrode materials, one of them is to combined both preferred properties of carbon based nanomaterials which provided high specific surface area and pore volume lead to high specific capacitance such as carbon nanotube (CNT) and the various metal oxides with obtained high energy density such as copper oxide nanowires (CuO NWs) as a so-called hybrid electrode materials. Although many synthesis methods have been investigated for example, thermal oxidation process and CVD method have been used to growth CuO NWs/CNT nanocomposites but it is still lack information corresponding to their good properties of electrode materials especially at the atomic level. Here, the structural and electrochemical properties of CuO NWs are investigated using density functional theory with Hubbard U corrections (DFT+U), followed by the investigation of a number of different low index CuO surfaces. The stabilities, electronic structure and electrochemical properties are presented. CuO (111) and (_111) were found to have the lowest surface energies which is good agreement with the XRD pattern of CuO NWs. We consider the pathways for growing of CuO NWs by studied the oxygen vacancies formation and oxygen molecule adsorption on two most exposed CuO surfaces will be discussed.

Primary author: Dr PHONYIEM, Mayuree (College of Nanotechnology, King Mongkut's Institute of Technology Ladkrabang)

Presenter: Dr PHONYIEM, Mayuree (College of Nanotechnology, King Mongkut's Institute of Technology Ladkrabang)

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