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Bulk, Surface and Catalytic Properties of Metal Carbides: A Systematic DFT Study

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For this presentation, I will discuss the results of a comprehensive study into the bulk and surface properties of all available transition metal carbides with rock-salt structures. I will explain how the bonding character of the materials is dependent on the periodic position of the transition metal and the direction of the surface termination, which in turn tunes the density of states and surface properties. Special consideration will be given to the possible catalytic implications of these surface properties on CO_2 hydrogenation.

The development of chemical processes that utilize CO_2 as a cheap feedstock in the production of valuable chemical is considered by many as a very importance precursor to the future development of a low-carbon economy. Therefore, a primer focus of this current study is to compare those aspects of transition metal carbides that impact on their future usefulness as catalysts in the conversion of CO_2. To this end, the work that i will present in this conference severs as a comprehensive screening of the electronic and catalytic properties of many different carbides. The knowledge gained from this study is forming the basis for our current work into the conversion of CO_2 using photo-generated hydrogen.

Biography:

Matthew George Quesne completed his undergraduate at the University of Lancaster (United Kingdom) with specialization in Biochemistry. He then moved to the University of Manchester to pursue his PhD studies under the supervision of Dr Samuel de Visser in the field of enzyme catalysis. He was awarded his PhD in 2014 and joined the research group headed by Dr Tomasz Borowski at the Institute of Catalysis and Surface Chemistry, Polish Academy of Science Krakow (Poland). In April 2016, he moved to Cardiff University to work in the group of Prof. Richard Catlow, where he is investigating CO_2 activation on transition metal carbides.