Research project and supervisory team

Supervisory Team	Dr. Hainam Do; Prof. Jim Greer
Short introduction & description of research project	This PhD project will focus on materials computational modelling for chemical sensing. Highly motivated students with a degree in chemical engineering, chemistry, physics, or material science are encourage to apply. This project is part of a larger programme between the Departments of Chemical Engineering, Computer Science and Electrical and Electronic Engineering leading to intelligent sensors. Chemical sensing, as are sensors in general, are now in use for a wide range of applications in chemistry, energy, industrial control, and health applications. For example, there are typically between a half dozen to two dozen sensors performing different tasks in a modern smartphone, allowing information from the external world to be converted to digital information for processing and decision making. Often information from a large number of sensor nodes in a network is transmitted to a central computing infrastructure such as the 'cloud' or a locally dispersed computing infrastructure (the 'fog'). In the era of IoT and big data, the requirements for gas sensors, in addition to sensitivity and selectivity, have been increasingly placed on sensor simplicity, deployment in 'dirty' environments, ease for integration, and flexibility. A key to meet these requirements is the development of high-performance gas sensing materials. Two-dimensional (2D) materials provide a number of attractive properties that are beneficial to gas sensing, including the versatile and tuneable electronic/optoelectronic properties, the rich surface chemistry and they can be readily convert chemical detection into electrical signals. Since the materials are '2D', the surface-to-volume ratio is exceptionally high, allowing for chemical detection to readily modulate electronic currents, hence providing an efficient transducer. Understanding the gas-solid interaction and the subsequent signal transduction pathways is essential for improving the performance of existing sensing materials and searching for new high performing materials. In this project, the reactivity for flammable (butane, hydrogen, propane, methane) and toxic (carbon monoxide, sulfur dioxide) gases interacting with various low-dimensional structures will be investigated using quantum chemical calculations to determine reactivity and bonding mechanisms to the sensor materials. Since quantum confinement effects strongly influence the electronic structure of nanostructures, tailoring the geometries to induce a significant perturbation upon specific gas absorption to the band structures will be explored.
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