

SINGA Awards – IHPC Projects

Name:	Dr Wu Ping	Programme :	Computational Materials Science and Engineering
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Research Area/ Theme			
<p>Materials Science: Dr. Wu Ping is interested in materials design and development through a combined approach of computer modelling and experiment. Over the last 10 years, a set of multiscale computational techniques has been set up for simulation of materials chemical behaviours in systems from as small as a few atoms to tones in mass and for actions those last from as short as pico seconds to hours or even years. Three modelling approaches (quantum chemistry, thermo-chemistry and datamining/artificial intelligence) are integrated successfully to provide a common platform for research and teaching in materials science. Fundamental relationships among chemistry, materials structure, chemical processing, and product properties, are established for many important materials systems like multicomponent oxides, semiconductors, and alloys.</p>			
Proposed Project Title:	Study of advanced multifunctional semiconductors		
<p>This project aims to develop new understanding and fundamental mechanism that govern the electronic, magnetic and optical properties of semiconductors, through multiscale computer modelling and experiment. We are keen on ZnO, NiO, BaTiO₃, PbTiO₃, and Ge-Sb-Te (GST) based materials which showing coupled functions like multiferroics, electro-optics, and phase change magnetism. We also design new semiconductors of multifunctional nature.</p>			
Proposed Project Title:	Novel materials for fuel cells and energy storage applications		
<p>We focus on the design of new cathode materials for Solid Oxide Fuel Cells (SOFC), Polymer Electrolyte Membrane Fuel Cells (PEMFC), and anode for Li-battery. In SOFC research, energy band structure and the effect of electron-correlation in transition metal oxides to electrochemical reactions are studied. The obtained new knowledge will be used to guide in the design of new cathode materials. To reduce the cost of PEMFC, new structures of non-noble transition metal-organic complex will be designed to replace Pt cathode. In the Li-battery research, we design a new CNT-Sn nanostructure to increase the anode stability.</p>			