

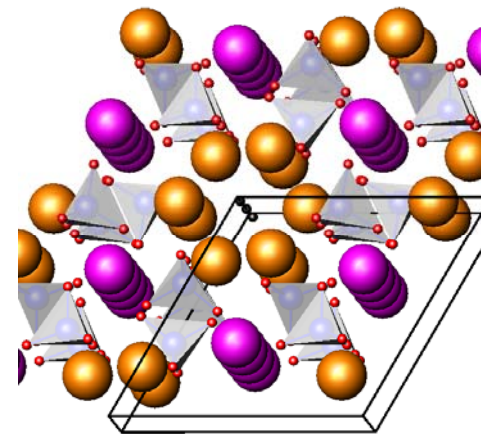
# FYP Research Projects on Nano-Structured Functional Materials

---

**Dong Zhi-Li**

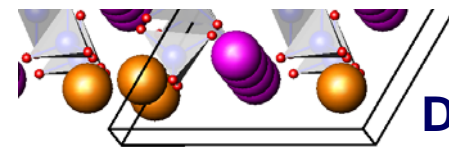
**School of Materials Science & Engineering,  
Nanyang Technological University, 50 Nanyang  
Avenue, 639798 Singapore**

**E-mail: [zldong@ntu.edu.sg](mailto:zldong@ntu.edu.sg)**



# Tentative FYP Projects: 2011-2012

- Crystal Structure and Properties of Hydrothermally Synthesized Zinc Oxide (A\*STAR-MSE joint project)
- Facile Synthesis of Metal Oxide for Photocatalytic Applications
- Atomistic Simulation of Carbon-based Nano-materials (A\*STAR-MSE joint project)
- First-principles Study of Ionic Conductor  $\text{Li}_3\text{N}$  (ASTAR-MSE joint project)
- Microstructure and Mechanical Properties of Nano-Composites
- Experimental Study on Mechanical/Electrical Properties of CNT Containing Nanomaterials
- On the heat distortion temperature of PLA-based nanocomposites
- New: Advanced waste gasification/pyrolysis for bio-energy production (MSE-iESE joint project)

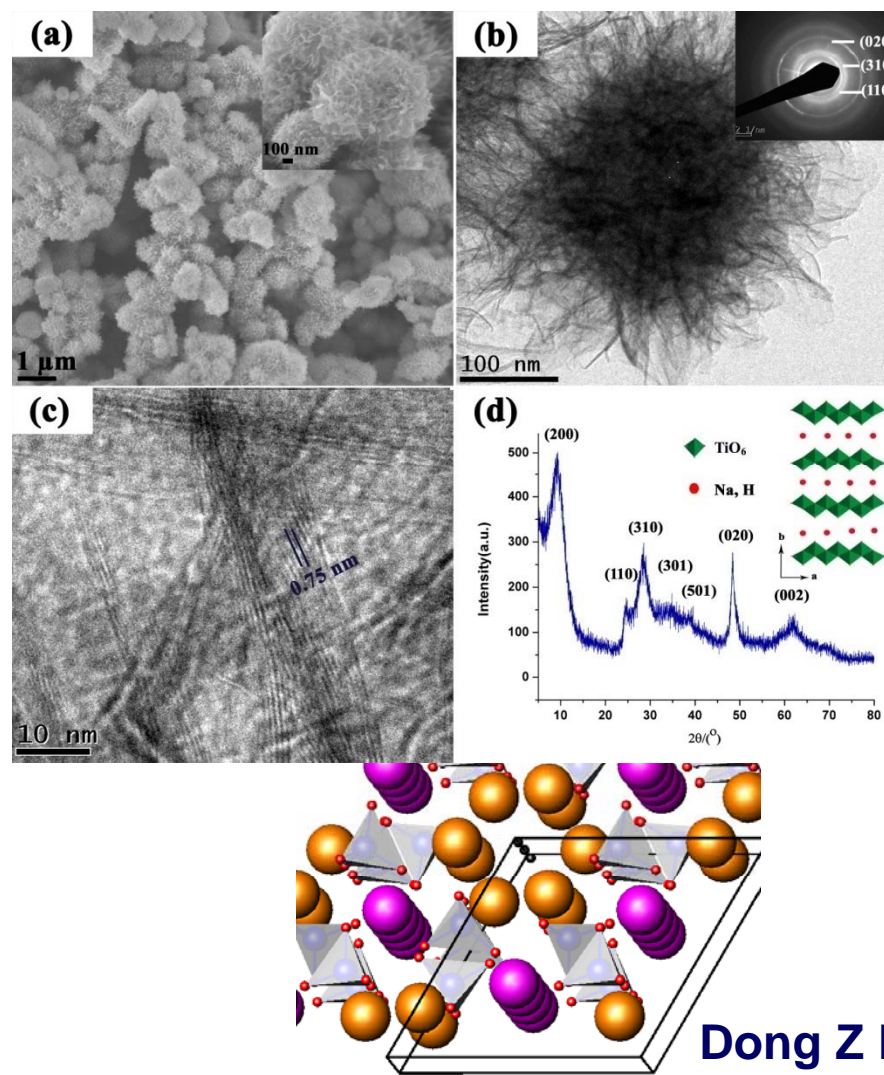


Dong Z L

# Facile Synthesis of Metal Oxide for Photocatalytic Applications

In our previous work, one-step approach is applied to quickly fabricate layered titanate hierarchical microparticles.

In this project, students will apply this technique to fabricate different metal oxides and test their photocatalytic properties.



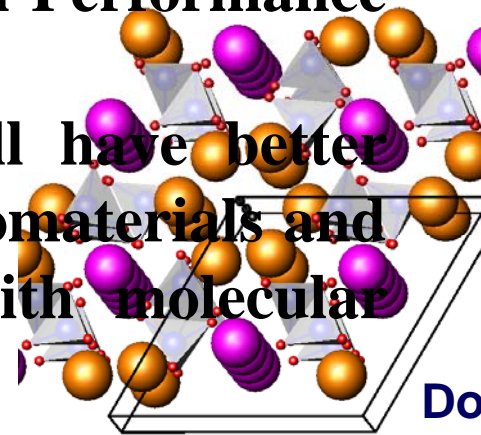
# Atomistic Simulation of Carbon-based Nanomaterials

---

In this final year project, atomistic simulation will be used to study the mechanical and thermal properties of carbon-based nanomaterials. The project work will include constructing the simulation models for the nanomaterials, and then performing molecular dynamics simulations under different loading and boundary conditions.

The simulations will be carried out on the supercomputers at the Institute of High Performance Computing (IHPC), A\*STAR.

Through this project, the student will have better understanding of the properties of nanomaterials and at the same time be well trained with molecular dynamics simulation.

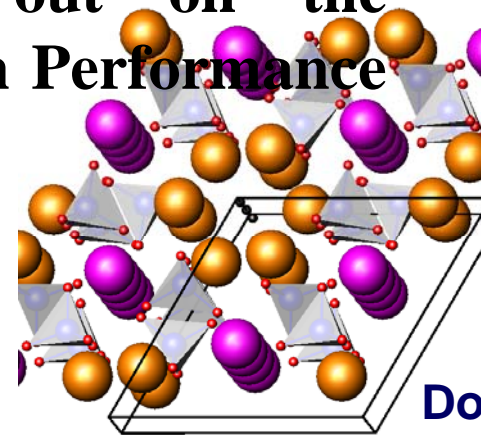


Dong Z L

# First-principles Study of Ionic Conductor $\text{Li}_3\text{N}$

Fast Li ionic conductor  $\text{Li}_3\text{N}$  has potential application as solid electrolyte in Li-ion rechargeable batteries. Its ionic conduction is dependent on Li vacancies. Ready commercial software VASP will be applied to calculate Li vacancy formation energy, which will help understand the relationship between structure and ionic conduction.

The simulations will be carried out on the supercomputers at the Institute of High Performance Computing (IHPC), A\*STAR.



Dong Z L