BỘ MÔN TIN HỌC VẬT LÝ, KHOA VẬT LÝ,
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Seminar

Date: Friday 05th Oct. 2018 / Time: 9:00 am – 10:00 am / Place: Room 408F, Building T1

Campus: 334 Nguyễn Trãi, Thanh Xuân, Hà Nội

Kính mời thầy cô và các bạn quan tâm đến dự / Everyone is welcome !

Speaker: Dr. DINH VAN AN (JICA long-term Expert at Nanotechnology Program, Vietnam Japan University, VNU; Graduate School of Engineering, Osaka University, Japan)

Title: COMPUTATIONAL MATERIAL DESIGN FOR ION BATTERIES AND ORGANIC GAS SENSORS

Abstract: In this talk I will introduce two research directions of my group:

1. **Material design for rechargeable ion batteries**: Using the density functional calculations, we investigated the crystal and electronic structures, electrochemical properties and ion diffusion mechanism of several materials used for cathode and anode of Li/Na ion batteries. The diffusion of Li+/Na+ ion which is accompanied by a positive small polaron is described by three elementary diffusion processes, including single, crossing and parallel diffusions [1]. Diffusion barrier and pathway are explored by NEB method.

2. **Material design towards the early detection of lung cancer**: Every year, the large number of death due to lung cancer is reported. 5 years after diagnosis, there are only 14% of the lung cancer patients are alive. Screening tests to detect lung cancer at an early stage is very important for localizing the cancer cells and significantly improving the possibility of the curability of the disease. Breath contains clinically useful markers such as the violate organic compounds (VOCs), which can be detected by electronic sensors. In this seminar, I will introduce briefly the quantum simulation methods in searching the 2-dementional materials for the sensitive devices that can be used in detecting the lung cancer at early stage.

References:

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2. *K. M. Bui,* ***V. A. Dinh****, and T. Ohno, Diffusion of polaron-Li complex in lithium silicate Li_2FeSiO_4, Appl. Phys. Express* ***12*** *(2012) 125802*.

3. *D. M. Duong,* ***V. A. Dinh*** *and T. Ohno, Quasi-3D diffusion of Li ions in carbonophosphate $Li_2Fe(PO_4)_3CO_3$. Appl. Phys. Express* ***6*** *(2013) 115801*.

4. *K. M. Bui,* ***V. A. Dinh****, S. Okada and T. Ohno, Hybrid functional study of the NASICON-type $Na_3V_2(PO_4)_3$: Crystal and electronic structures, and polaron-Na vacancy complex diffusion. Phys. Chem. Chem. Phys.* ***17*** *(2015) 30433.*

5. *K. M. Bui,* ***V. A. Dinh****, S. Okada and T. Ohno, Diffusion in NASICON-type electrolyte material NZSP for all-solid-state batteries: Density functional study. Phys. Chem. Chem. Phys.* ***18*** *(2016) 27226.*

6. *M. Debbichi, L. Debbichi,* ***V. A. Dinh*** *and S. Lebègue, First principles study of the crystal, electronic structure, and diffusion mechanism of polaron-Na vacancy of $Na_3MnPO_4CO_3$ for Na-ion battery applications. J. Phys. D: Appl. Phys.* ***50*** *(2017) 045502*.

7. *H. D. Luong, Y. Morikawa, Y. Shibutani and* ***V. A. Dinh****, Difusion mechanism of Na ion – polaron complex in potential cathode in potential cathode materials NaVOPO4 and VOPO4 of rechargeable sodium-ion batteries. Phys. Chem. Chem. Phys.* ***20*** *(2018) 23625.*

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