CURRENT SITUATION OF OF MATERIALS RESEARCH IN HCM CITY UNI. OF TECHNOLOGY, (HCMUT) VIETNAM



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1.1. GENERAL DESCRIPTION OF HCMUT

- one of the oldest and the most prestigious higher education institution in the South of Vietnam
- founded in 1911 by the French colonial administration
- subsequently named by:
- 'National Technical Center' in 1957,
- 'National Technical Institute' in 1972,
- 'Polytechnic University' in 1976, and
- by the present named HCMUT from 1993
- Nowadays, it constitutes one of three colleges of the
- "Vietnam National University of HoChiMinh City".
- The other two colleges are the College of Natural Sciences and College of Human Sciences

1.2. MAJOR ACTIVITIES

- a) education and training of civil engineers and graduates at different levels up to Master and Ph.D.degrees;
- b) scientific research and transfer of scientific and technological expertise and innovation to the enterprises and industries, and in general to the society,
- c) collaboration with international partners for the high-level training and transfer of technology.

1.3. CAPACITIES

- composed of 11 faculties, 61 departments in total
- having 25.000 undergraduate students and about 1500 graduate students.

HCMUT FACULTIES:

- 1) FACULTY OF APPLIED SCIENCE
- 2) FACULTY OF CIVIL ENGINEERING
- 3) FACULTY OF CHEMICAL ENGINEERING
- 4) FACULTY OF ELECTRICAL AND ELECTRONICS ENGINEERING
- 5) FACULTY OF INFORMATION TECHNOLOGY
- 6) FACULTY OF ENVIRONMENTAL ENGINEERING
- 7) FACULTY OF GEOLOGY AND PETROLEUM
- 8) FACULTY OF INDUSTRIAL MANAGEMENT
- 9) FACULTY OF MECHANICAL ENGINEERING
- 10) FACULTY OF MATERIALS TECHNOLOGY
- 11) FACULTY OF TRANSPORT

1.4. CLUSTER SYSTEM

- Hardware view
- Total system includes 01 Master node, 64 compute nodes. All nodes are used 2 links for communicating. The first link is Fast Ethernet for monitoring purposes. The second is Gigabit Ethernet for computing data.
- Computing node configuration

 Dual Xeon 2.8GHz Hyper Threading; 1GB ECC

 DDRAM, 40GB HDD; 02 Gigabit Ethernet ports.
- Master node configuration
 Dual Xeon 2.4GHz Hyper Threading; 2GB ECC
 DDRAM, 40GB HDD; 02 Gigabit Ethernet ports.
 01 Fast Ethernet port.

- Software view
- The operating system on nodes is RedHat Enterprise Workstation 3.0.
- -Compilers: Gnu C/C++, Fortran 77, Java. Version 3.2, Intel C/C++, Fortran Compiler.
- For parallel programming, MPI libraries: LAM/MPI 7.0.4; MPICH 1.2.5.2; PVM 3.4.3-6
- -- MATH and other libraries: BLAS, ATLAS, BLACS, LAPACK and SCALAPACK.
- The PBS queuing and Maui scheduler system to support user submitting their jobs.
- Applications: ANSYS, GAUSSIAN, MATLAB, WIEN2K, GULP, VSAP, ...



INTRODUCTION TO FACULTY OF MATERIALS TECHNOLOGY

HISTORY:

Founded in June 2001 by unifying three branches:

- Polymer Materials and Silicate Materials from the Faculty of Chemical Engineering
- Metallic Materials from the Faculty of Mechanical Engineering

FACILITIES:

- building: block C4
- 4 laboratories belongs to 4 departments and 1 central laboratory belongs to the faculty
- 4 departments
- 3 research centers: polymer materials research center, silicate materials research center and new materials research center

DEAN BOARD:

Dean: M.Eng DO THANH THANH SON

Vice Dean: Dr. NGUYEN THANH LOC

STAFF: (43 persons)

3 Professors, 10 Doctors, 11 M.Eng, 17 B.Eng

STUDENTS: (736 Students in total)

MATERIAL SCIENCE **METALLIC MATERIALS FUNDAMENTALS TECHNOLOGY DEPARTMENTS POLYMER SILICATE**

MATERIALS
TECHNOLOGY

SILICATE MATERIALS TECHNOLOGY

MATERIAL SCIENCE FUNDAMENTALS



STAFF:

01 Professor 05 Doctors 05 B.Eng

LAB: 02

Basic Material Science Lab.

Corrosion & Surface Treatment Lab

RESEARCH ORIENTATIONS:

Advanced Materials

Corrosion protection & Electrochemical Engineering

Fuel Cells

METALLIC MATERIALS TECHNOLOGY

LAB: 01
Metallic Materials
Technology

STAFF: 01 Professor 03 Doctors 04 M.Eng 05 B.Eng.

RESEARCH ORIENTATIONS:

- Sintered alloys
 - Metallurgy
 - Casting
- Heat treatment
- New materials

POLYMER MATERIALS TECHNOLOGY

STAFF:

01 Professor 01 Doctor 06 M.Eng 02 B.Eng.

LAB: 01

Polymer Materials Technology Lab.

RESEARCH ORIENTATIONS:

- Special Polymers
- Composite Materials
- High Performance Polymers
- Polymer Blend



3. Group of Computation

3.1. MEMBERS

Dr. Pham Thanh Quan, Faculty of Chemical Engineering Dr. Nguyen Thanh Loc, Faculty of Materials Technology MSc. Le Thanh Hung, Faculty of Chemical Engineering Pham Ho My Phuong, PhD. stud., Univ. of Utah, USA Nguyen Thanh Lam, PhD. stud., Univ. of Leuven, BEL. Huynh Kim Lam, PhD. stud., Univ. of Utah, USA Nguyen Giao Hoa, PhD. stud., Univ. of Utah, USA Nguyen Kim Trung, Faculty of Chemical Engineering **Master Students**

3.2. MAIN RESEARCH AREAS

- Pollution in Atmosphere (atmospheric chemistry, combustion reactions ...)
- Structures and properties of nanomaterials (nanotubes, nanowires, nanoparticles ...) and catalyst (zeolite, homogenous and heterogeneous catalyst ...)
- Properties of materials (metals, semiconductors, polymers, mineral oxides ...)
- Structures and reactivity of organic/biological molecules
- Decomposition rules of substrates in mass spectrometry

3.2. MAIN RESEARCH AREAS (ctn.)

- Development and application of chemical reactivity indexes in explaining and predicting reaction mechanism by Density Functional Theory.
- Kinetics and Mechanism of polymerization reactions in gas phase, cycloaddition reactions, combustion reactions, hydrogenation and dehydrogenation reactions.
- Theoretical calculation of thermodynamic quantities such as equilibrium constants, reaction rates, heat of formation, proton affinity, electronegativity ...
- Process simulation and modellization

International Cooperation

- University of Leuven, Belgium, Prof. Nguyen Minh Tho, Prof. Arnout Ceulemans
- University of Brussels, Belgium, Prof. Paul Geerlings, Prof. Frank De Proft
- University of Hyderabad, India, Prof. Kalidas Sen
- University of North-Eastern Hill, Dr. Asit Kumar Chandra
- University of Utah, United States, Prof. Truong Nguyen Thanh
- University of Fisk, United States, Prof. Lawrence M. Pratt

3.3. RECENT PUBLICATIONS (2002 - now)

- 1) A theoretical approach to the regioselectivity in 1,3-dipolar cycloadditions of diazoalkanes, hydrazoic acid and nitrous oxide to acetylenes, phosphaalkynes and cyanides.
- Loc Thanh NGUYEN, Frank De PROFT, Van Luong DAO, Minh Tho NGUYEN and Paul GEERLINGS.
- Journal of Physical Organic Chemistry, 2003, 16, 615 625.
- 2) Regio- and stereoisomeric composition of the product mixture in the Diels-Alder reaction of dicyclopentadiene with bicyclononadiene: a NMR and DFT quantum chemical investigation.
- Monique BIESEMANS, Hassan DALIL, Loc Thanh NGUYEN, Bart HAELTERMAN, Ghislain DECADT, Francis VERPOORT, Rudolph WILLEM and Paul GEERLINGS.
- Tetrahedron, 2002, 58, 10447 10453.
- 3) Local Softness versus Local Density of States as Reactivity Index.
- Loc Thanh NGUYEN, Frank De PROFT, Montserrat Cases AMAT, Gregory VAN LIER, Patrick W. FOWLER and Paul GEERLINGS.
- Journal of Physical Chemistry A, 2003, 107, 6837 6842.

- 4) Protonation and Methylation of Thiophenol, Thioanisole and their Halogenated Derivatives: Mass Spectrometric and Computational Study. P. C. NAM, R. FLAMMANG, H. T. LE, P. GERBAUX and M. T. NGUYEN. International Journal of Mass Spectrometry, 228, 151 165 (2003).
- 5) Molecular and Electronic Structure of Zwitterionic Diamino-Meta-quinonoid Molecules.
- H. T. LE, P. C. NAM, V. L. DAO, T. VESZPREMI and M. T. NGUYEN. Molecular Physics, 101, 2347 2355 (2003).
- 6) Density Functional Study of the Decomposition Pathways of Nitroethane and 2- Nitropropane.
- P. A. DENIS, O. N. VENTURA, H. T. LE, M. T. NGUYEN. Physical Chemistry Chemical Physics, 5, 1730 1738 (2003).
- 7) 1,4 Nitromethane Methyl Nitrite Rearrangement: A Persistent Discrepancy between Theory and Experiment.
- M. T. NGUYEN, H. T. LE, B. HAJGATO, T. VESZPREMI and M. C. LIN. Journal of Physical Chemistry A, 107, 4286 4291 (2003).

- 8) 4,4-p-Biphenyl bis-Phosphinidene: Generation of a bis-W(CO)5 Complex and Ab-initio Calculation of its Electronic Structure.
- N.H. TRAN-HUY, H. T. LE, F. MATHEY and M. T. NGUYEN. Journal of Chemical Society, Perkin Transactions 2, 2140 2145 (2002).
- 9) Ionized Aniline and Its Distonic Radical Cations Isomers.
- H. T. LE, R. FLAMMANG, M. BARBIEUX-FLAMMANG, P. GERBAUX and M. T. NGUYEN.
- International Journal of Mass Spectrometry, 217, 45-54 (2002).
- 10) Collisional Induced Loss of NO₂ Radical from Protonated Nitroimidazoles and Nitropyrazoles.
- R. FLAMMANG, J. ELGUERO, H. T. LE, P. GERBAUX and M. T. NGUYEN. Chemical Physics Letters, 356, 259 266 (2002).

MATERS THESIS

- 1) Mechanism and Kinetics of Chain Transfer and Back-Biting Reactions in Polyethylene Addition, Nguyen Thi Thu Cuc, presented in 7/2004 at HCMUT.
- 2) Kinetics of 1, 3 Hydrogen Shift of Alkyl Radical Reaction Class: An Application of the Reaction Class Transition State Theory, Pham Ho My Phuong, presented in 7/2004 at HCMUT.
- 3) Mechanisms of Diels-Alder Cycloaddition Reactions of Substituted Butadienes and Ethylenes, Do Quy Diem, presented in 1/2005 at HCMUT.

3. Some remarks

What we will have:

- At the end of 2007 we will have some equipments for materials characterization: FE-SEM-Xray Microanalysis, AFM, Spectrum Analyzer, Dilatometer...
- Lab. of Nanomaterial technology (HCM National University)

What we need:

- Training for operating, maintenance of equipments
- Experience in doing researches in materials technology

