Introduction of the Dalian Institute of Chemical Physics (DICP), CAS

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  - the State Key Laboratory of Catalysis (SKLC)

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  - Nano-pore: Confinement effects
中国科学院大连化学物理研究所
Dalian Institute of Chemical Physics, CAS

Dalian
1hr from Beijing
About the Chinese Academy of Sciences

**STRUCTURE:**

- **Merit-based Academic Divisions:**
  - Members: 700 inc.
  - 35 Foreign Members

- **Comprehensive National Research Institution:**
  - 90 Institutes,
  - 1 University
  - 1 Postgraduate School
  - Total Staff: 50,000

**MISSIONS:**

- Scientific Research
- High Technology Development
- Education and Training
- Think Tank of Science Policies
Dimensions of Dalian Institute

Staff Members

- Academ
- Prof.essor
- Assoc. Pr.of
- M dd.
- Pr.im
- Post doc.
- Student s

Graduate Students

- 51 Research Groups and Teams
- 1500 Researchers
Research Organizations of DICP

Basic Research

- State Key Laboratory of Catalysis
- State Key Laboratory of Molecular Dynamics

National Key Projects

- Laboratory of Fuel Cell
- Laboratory of Chemical Lasers
- Laboratory of Materials

Applied Research

Spin-off Companies

- Pesticide Intermediates
- Membrane Technology
- Chromatographer
- Fuel Cell
- Catalyst
Fundamental Researches at DICP

Science 2
Nature 1
Agew. Chem 7
JACS & PRL 11

1 National Science Award
2 National Invention Award
Fundamental Researches in DICP


Quantized Transition States

Science, March 2006
Applied Researches in DICP

- Sustainable Energy
- Resources Optimal Utilization
- Bio-Technologies
Energy Researches in DICP

- **Optimal Utilization of Natural Gas**
  - Production of Syngas via Low-cost Process
  - Syngas Chemistry including FT and Oxygenate Synthesis
  - Direct conversion of Methane

- **Hydrogen Energy**
  - Hydrogen Production from Natural Gas, Lower Alkanes and Resid as well as Methanol
  - Hydrogen Production via Bio-technology
  - Separation of Hydrogen from Carbon Monoxide and Carbon Dioxide by membranes

- **Fuel Cell**
  - Proton-Exchange Membrane Fuel Cell (PEMFC)
  - Solid Oxide Fuel Cell (SOFC)
  - Direct Methanol Fuel Cell (DMFC)
  - Micro Fuel Cell and Micro Sensors
Key Techniques to Polygeneration

- **Chemical Synthesis**
- **WGS**
- **S resistant**
- **Gasifier**
- **Cleaning**
- **SOFC**
- **Methanol**
- **Diesel**
- **Olefins**
- **Ethanol**
- **Separation**
- **Storage**
- **Fuel Cell**
- **Oxygen**
- **H2**
Utilization of Natural Gas & Coal

Resources

Gas
Methane

Coal/Bio-
Future?

Products

Fuel Cell
SOFC

Benzene, H2

Ethylene, Propylene

Alcohols, Ethers,

Gasoline, Diesel

Syngas

H2 CO₂ Cap.

Methanol

含氧化合物

芳香烃和氢

烯烃
Gas to Liquid (GTL)

Syngas
- Coal-based
  - Fe
  - Gasoline, Diesel
    - ICC

Syngas
- Gas-based
  - Co
  - Diesel, Waxes

Pilot test in Ningbo
C2 Oxygenates from Syngas

Coal & Gas

CO + H₂ → CO Conv. 56.4%
Selec. 73.5 wt%

C₂ Oxygenates

EtOH

Hydrogenation

Oxygenation

AcOOH

AcOOEt

Economic. (BP):
Present Tech. 2500 ~ 2800 RMB/ton Eth.
The unique pore size allows the selective conversion to olefins and excludes heavier compounds.
Pilot and Demo of the MTO process

- Shanxi Coal Company (86 million RMB)
- Sinopec Leyang Eng. Comp. (Tech Design)
- DICP (Catalyst & Process)

Diagram with data points and lines on a graph showing conversion rate and selectivity. The graph includes temperature axes labeled in度C (°C).
Dimethyl Ether (DME) and its Manufacture

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting Point (°C)</td>
<td>-141</td>
</tr>
<tr>
<td>Vaporization Heat (-20°C, KJ/Kg)</td>
<td>410.2</td>
</tr>
<tr>
<td>Boiling Point (0.1 Mpa, ℃)</td>
<td>-24.8</td>
</tr>
<tr>
<td>Autoignition Temperature (℃)</td>
<td>235</td>
</tr>
<tr>
<td>Critical Pressure (MPa)</td>
<td>5.37</td>
</tr>
<tr>
<td>Critical Temperature (℃)</td>
<td>126.9</td>
</tr>
<tr>
<td>Critical Density (Kg/m³)</td>
<td>0.271</td>
</tr>
<tr>
<td>Ignition Temp (℃)</td>
<td>-41</td>
</tr>
<tr>
<td>Specific Gravity</td>
<td>1.59</td>
</tr>
<tr>
<td>Calorific Value (MJ/Kg)</td>
<td>31.75</td>
</tr>
<tr>
<td>Density (0.5Mpa, Kg/m³)</td>
<td>670</td>
</tr>
<tr>
<td>生成热 (KJ/mol)</td>
<td>-183</td>
</tr>
</tbody>
</table>

(Direct)

Coal & Gas (CH4) → H2 → Syngas → Methanol (CH3OH)

(Indirect)

Syngas → CO → (Dehydro)
“Poly-DME-DMM”_Diesel Substitution

DME
Dimethoxymethane (DMM)
Dimethyldioxymethylene (DMM₂)
Poly-Dimethoxymethane (DMMₓ)

DMM₃₋₈

- Most suitable DME analog
- Can be blended with diesel without engine modifications
- Low emissions in engine testing
- Made from methanol, DME and formaldehyde via low temperature catalytic distillation reactor with acidic catalyst

<table>
<thead>
<tr>
<th></th>
<th>DMM</th>
<th>DMM₂</th>
<th>DMM₃₋₈</th>
</tr>
</thead>
<tbody>
<tr>
<td>BP, °F</td>
<td>42</td>
<td>105</td>
<td>152-315</td>
</tr>
<tr>
<td>Flash Pt., °F</td>
<td>0</td>
<td>&lt;24</td>
<td>65</td>
</tr>
<tr>
<td>Cetane No.</td>
<td>28</td>
<td>41</td>
<td>76</td>
</tr>
</tbody>
</table>

PM and NOx Emissions of 7 test fuels

Source: DOE/SWRL
Hydrogen Related Researches in DICP

- Reforming of Methane, Methanol, Gasoline, Diesel
  - DICP
- CO₂ Sequester.
- Risk evaluation, Fundamental research, DICP
- Manufacture
- Storage
- Transformation
- Distribution
- Utilization
- Fuel cell Combustion
  - DICP, Shengli, Beijing companies
- Electric vehicle
  - Portable power
  - Distributed power station
  - DICP, Shengli, Tsinghua, Tongji
- No current research activity
- Metal hydrides, Shanghai, Beijing
- Carbon nanotube, Shenyang
- Metal polymer, DICP
Strategy of Bio-Technology in DICP

Platform of System Biology

Proteomics
Metabonomics
Interomics (action)

GC-MS-LC-NMR
Fingerprint of Meta. Prod.
Meta. Controlling & Networks
Metabonomics

Protein with DNA
Protein with RNA
Protein with Protein
Protein with Metabolic Products

Chinese Med.

Drug & Targets
Chem. Fingerprints
Bio. Fingerprints

Indu. BioTech

BioMass Conv.
Methane Activ.
Alga Energy

Bio-Materials

Cell Therapy
Stem Cell Eng.
Controlling Deliver
Biomass Utilization at DICP

Biomass
- Residue Harvesting
- Energy Crops

Cat.

Sugar Platform
- Enzymatic Hydrolysis
- Lignin Products

Products
- Fuels, chemicals
- Materials
- Heat & Power

Thermochem. Platform
- Pyrolysis
- Gasification

Biorefineries

Biodiesel from CAS

1MW BGPG Power Plant from CAS
Catalysis researches at DICP

- **Basic Research**
  - State Key Laboratory of Catalysis
  - State Key Laboratory of Molecular Dynamics

- **National Key Projects**
  - Laboratory of Fuel Cell
  - Laboratory of Chemical Lasers
  - Laboratory of Materials

- **Applied Research**
  - Laboratory of Analytical Chemistry
  - Laboratory of Fine Chemicals
  - Laboratory of Chemical Engineering
  - Laboratory of Applied Catalysis
  - Division of Bio-Technology
the State Key Laboratory of Catalysis (SKLC)

Academic Committee
   Chair: Prof. Michel Che
   Co-chairs: Prof. Mingyuan He
               Prof. Xinhe Bao

Director of SKLC
   Prof. Can Li

International Advisory Committee

Catalytic Chemistry
   Prof. Wenjie Shen

Nano & interfacial Catalysis
   Prof. Xinhe Bao

Molecular Catalysis & In-situ Studies
   Prof. Can Li

Membrane Catalysis & Catalytic Materials
   Prof. Weishen Yang

Organo-Inorganic Catalytic Materials
   Prof. Qihua Yang

Theoretical Catalysis
   Prof. Weixue Li

Cooperated with applied research labs.

- Laboratory for Environmental Catalysis and Technology
- Laboratory for Applied Catalysis and Natural Gas Conversion
- Laboratory for Fine Chemicals
- National Center for Catalytic Technology Development
The present research Activities

- **Energy Catalysis**
  Fuel Cell, Hydrogen production, C1 Chemistry, Photocatalysis,

- **Environmental Catalysis**
  NOx reduction, VOCs oxidation and
  ultra-deep desulfurization and denitrogenation

- **Catalysis for Fine Chemicals and Chiral Products**
  Asymmetric synthesis, selective oxidation and hydrogenation

- **Nanocatalysis and Advanced Catalytic Materials**
  Au, Ag and noble metals, CO oxidation

- **In-situ, dynamic, time-resolved characterizations**

- **Theoretical catalysis**
Catalyst Characterizations

- **In-situ characterization**
  - FT-IR, NMR, UV Raman, Laser Raman, TPSR, TGA-DTA, ...

- **Dynamics and kinetics**
  - PEEM, Time-resolved Spectroscopy, LISF, TPD-Mass, ...

- **Structures of real catalysts**
  - XRD, SEM, TEM, EDX, BET, ...

- **Atomic, molecular and nano scale**
  - Multi Nano-Probe, HREELS, XPS, AES, LEED,
UV Resonance Raman Spectroscopic Studies on Catalysis

Achievements: Example 1
Non-oxidative Aromatization of Methane

\[ 6\text{CH}_4 \rightarrow \text{Ben} \: + \: 9\text{H}_2 \; \text{Mo/ZSM-5} \]

Frustration chemicals

Eng.

Graph showing trend from 1993 to 2003.
Oxygen Production:
- 100% oxygen permeation selectivity
- High oxygen permeation
- Continuous production of oxygen

Membrane Reactor:
- Combining reaction and air separation into a reactor
- Increasing yield and selectivity by controlling oxygen species
- Being energy efficient and relatively safe to operate
- Avoiding formation of hot spots

Applications of Mixed Ion & Electron Conductivity Oxygen Permeable Membrane

- Oxygen depleted
- MIECM

Dense ceramic membrane with mixed oxygen ionic and electronic conductivity

- Partial oxidation of hydrocarbons
- Selective oxidation of hydrocarbons
- Oxidative dehydrogenation of hydrocarbons

Achievements: Example 3
Composition of the Research Projects

- Applied, 37%
- MOST, 20%
- NSFC, 16%
- CAS, 15%
- Fund for SKL, 12%

MOST: Ministry of Sci. & Tech.
CAS: Chinese Academy of Sciences

Applied, 37%
Fundamental, ~ 63%
Budgets for Research in past years

<table>
<thead>
<tr>
<th>Year</th>
<th>Million</th>
</tr>
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<tbody>
<tr>
<td>1999</td>
<td>7</td>
</tr>
<tr>
<td>2000</td>
<td>10</td>
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<tr>
<td>2001</td>
<td>13</td>
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<td>2002</td>
<td>16</td>
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<td>2003</td>
<td>19</td>
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<tr>
<td>2004</td>
<td>22</td>
</tr>
<tr>
<td>2005</td>
<td>22</td>
</tr>
</tbody>
</table>
Reseurches to be focused

- Scientific bases for renewable energy, environmental begin, human health and better life, and optimized utilization of resources
- Design and synthesis of more active and selective catalysts including based nano materials
- Essential correlation through heterogeneous, homogeneous and enzymatic catalysis. Biocatalysis may play more and more role in synthesis chemistry.
- In-situ, dynamic, spatial and time-resolved characterization together with theoretical calculation may eventually reveal the nature of catalysis and make catalysis a science.
- Catalysts with desired functions could be designed and synthesized based on the fundamental understanding.
DICP’s Activities in International Collaboration
Research Collaboration in DICP

- Dispatch and Acceptance of Researchers
  - Domestic and overseas Organizations

- Contract Researches
  - Domestic and overseas Enterprises

- Joint Projects
  - Domestic and overseas Enterprises

- Joint Research Centers
  - Universities and Enterprises
  - Government Organizations
International and National Research Organizations at DICP

State Key Laboratory
- State Key Laboratory of Catalysis
- State Key Laboratory of Molecular Dynamics

National Eng. Center
- Membrane Sci. & Tech.
- Catalysis
- Hydrogen and Fuel Cell

International Joint Labs
- China-France Joint Lab. on Catalysis
- CAS-BP Energy Innovation Laboratory (EIL)
- CAS-MPG Partner Groups
- DICP-Sumsung Joint Lab. on Fuel Cell
- DICP-Lilly Program on Analysis and Fine Chemicals
Collaboration with the Organizations in Europe

- Fuel Cell Testing, Safety and Quality Assurance
- Carbon Dioxide Capture via Hydrogen Energy Technology
- SOFC Stack Technology for Operation at 600°C
- Gene Technique with Uni. of Aarhus
- Oligosaccharides with TCM-denmark
- CAS-BP Clean Energy Program
- DICP-Cambridge Training Project
- Metabolomics for Traditional Chinese Medicine
- Catalysis
- Joint Lab of Catalysis with CNRS
- PEM Fuel Cell with Lund Institute of Technology
- Sino-Swedish Workshop on FC
- MPG-CAS Partner Group
- DFG-NSFC Fuel Cell Program
- DICP-BASF INCON project
- DICP-Bayer Project
Cooperation Partner between UCSB and DICP
Supported by NSF

THE PARTNERSHIP FOR INTERNATIONAL RESEARCH AND EDUCATION AT THE UNIVERSITY OF CALIFORNIA

ELECTRON CHEMISTRY AND CATALYSIS AT INTERFACES

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To Enhance Comprehensive Cooperation at DICP

- Special funds for international cooperation and exchange
  (1 million RMB per year for travel and accommodation, i.e. student, postdoctoral researcher)

- Special funds for scientific symposia in DICP
  (1 million RMB per year for scientific program & costs)

- Open grants and projects for joint research
Thank for Attention

Welcome to DICP