

Summer School on Surface Science & Catalysis
August 13-25, UCSB/USA



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

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<http://www.fruit.dicp.ac.cn>

Contents

- **Introductions**

- the Dalian Institute of Chemical Physics (DICP)
- the State Key Laboratory of Catalysis (SKLC)

- **Nano-Catalysis**

- Nano-film: Quantum well states
- Nano-Particle: Quantum size effects
- Nano-pore: Confinement effects

中国科学院大连化学物理研究所

Dalian Institute of Chemical Physics, CAS



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:

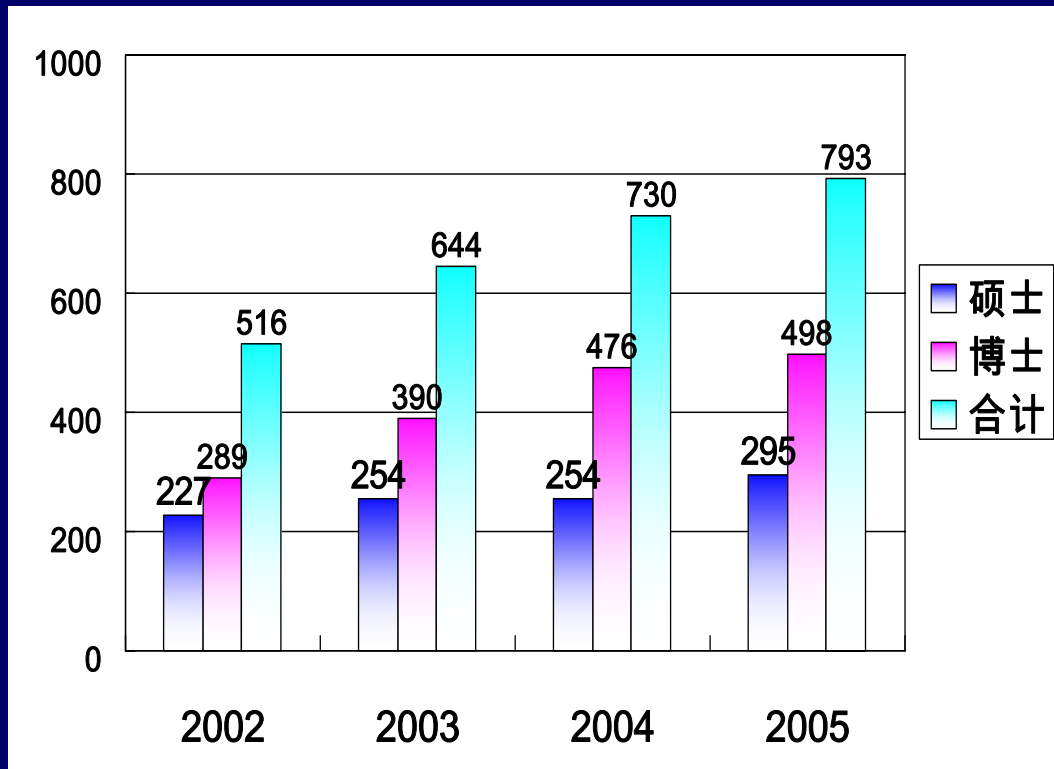
- **Scientific Research**
- **High Technology Development**
- **Education and Training**
- **Think Tank of Science Policies**

中国科学院大连化学物理研究所

Dalian Institute of Chemical Physics, CAS

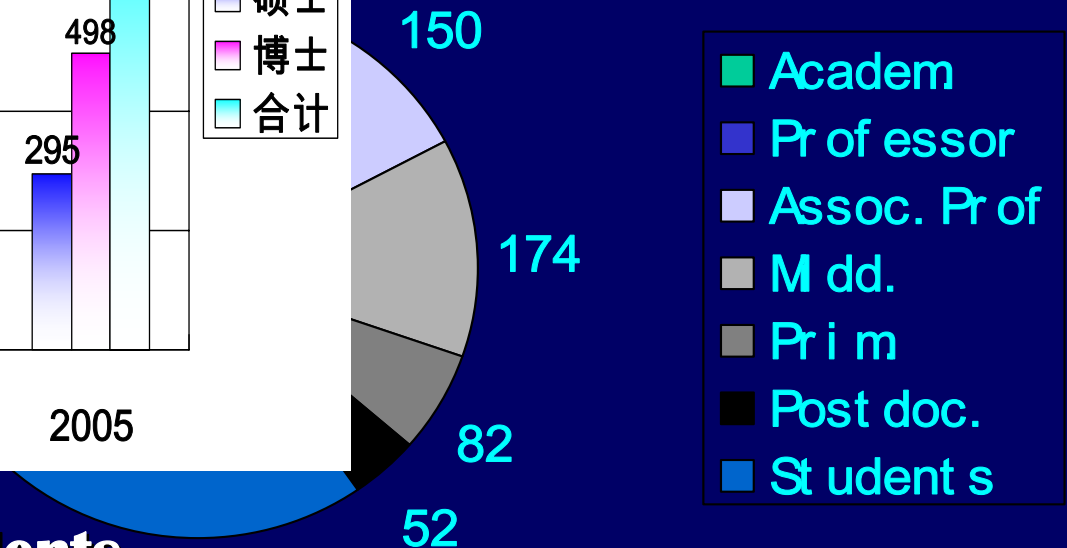


Dimensions of Dalian Institute



Graduate Students

Staff Members



● **51 Research Groups and Teams**

● **1500 Researchers**

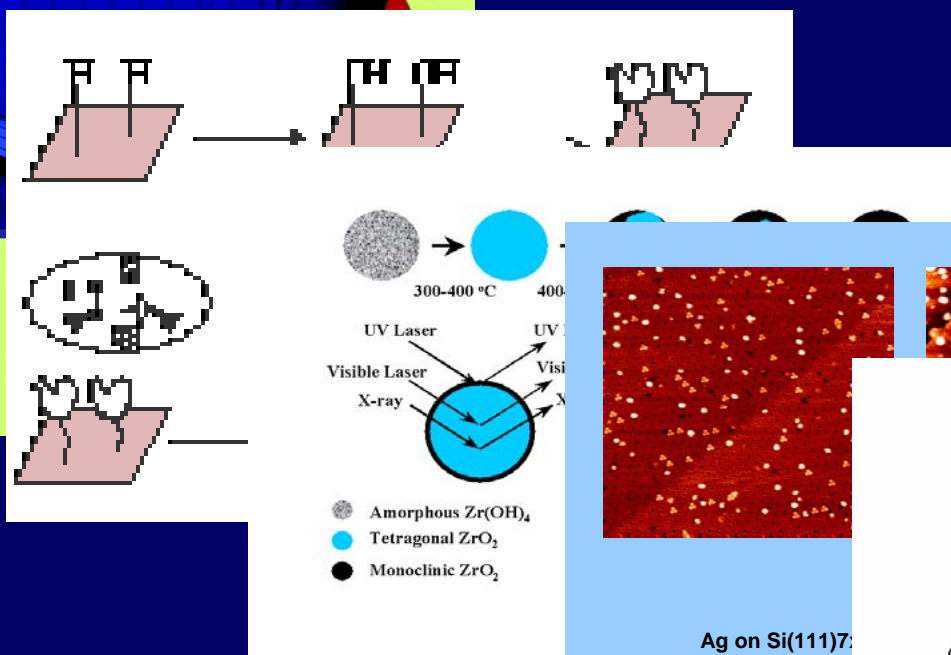
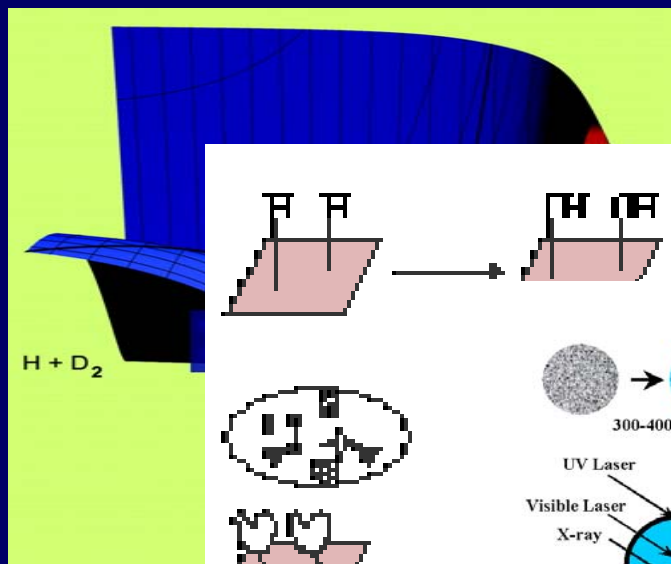
Research Organizations of DICP

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

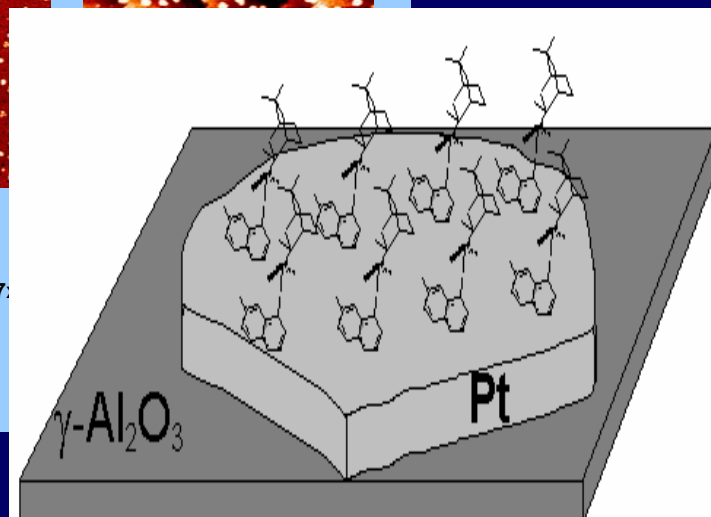
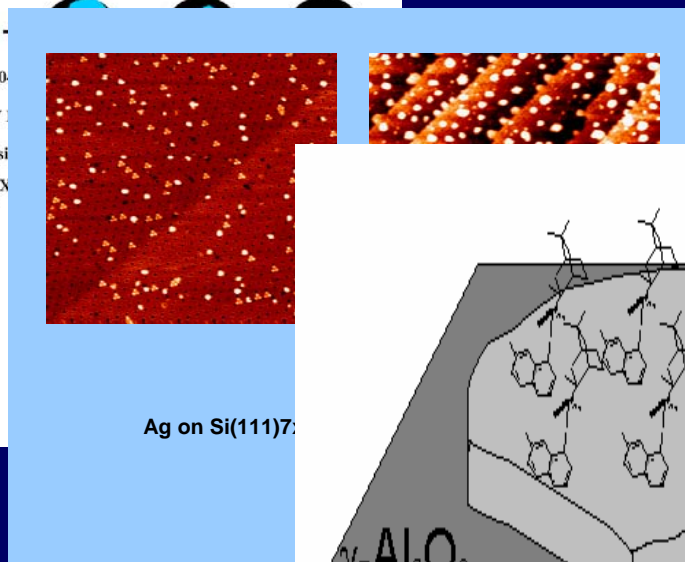
National Key Projects → **Laboratory of Fuel Cell**
→ **Laboratory of Chemical Lasers**
→ **Laboratory of Materials**

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

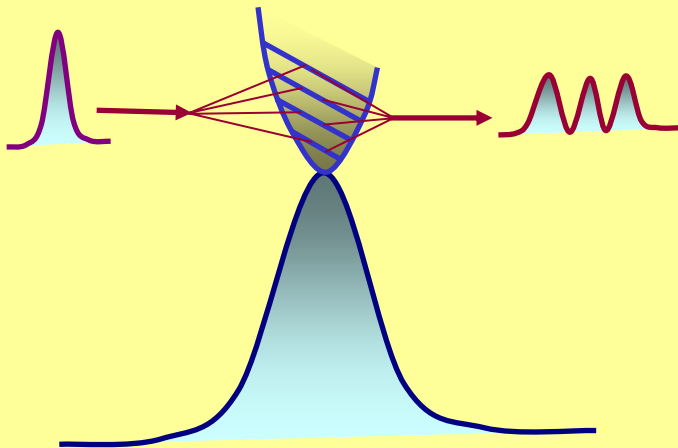


1 National Science Award
2 National Invention Award

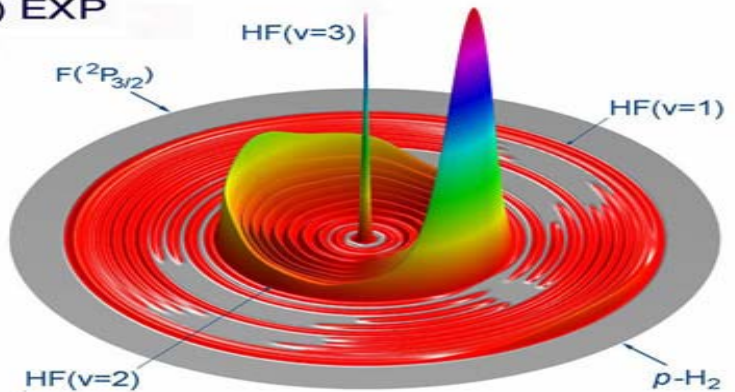
Fundamental Researches in DICP

Nature (2002)
Science (2003)

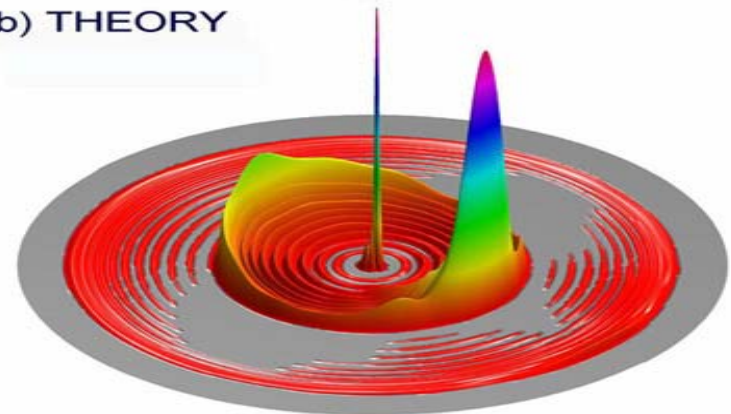
Quantized Transition States



a) EXP



b) THEORY



Science, *March 2006*

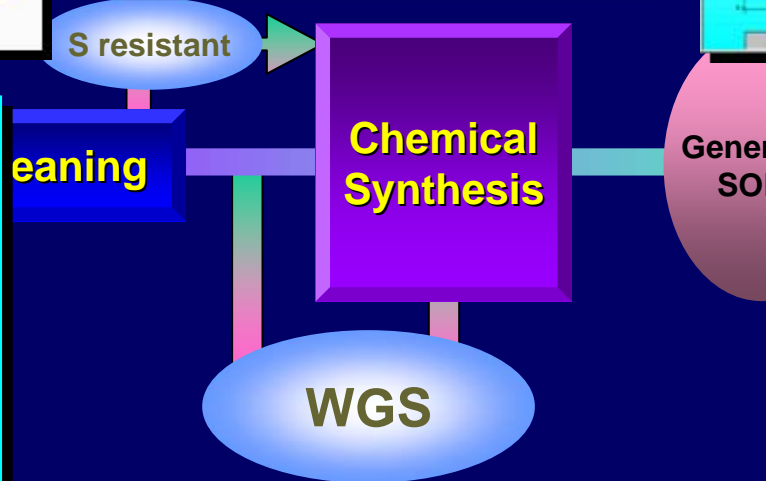
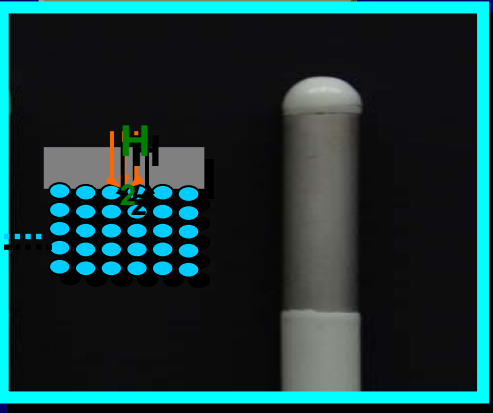
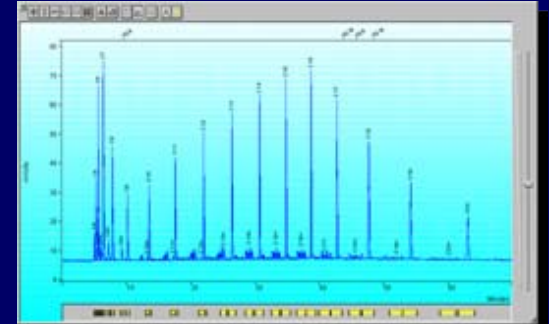
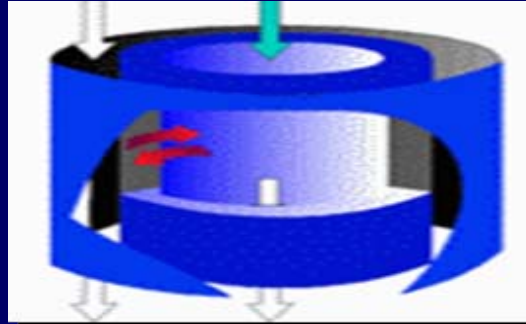
Applied Researches in DICP

- **Sustainable Energy**
- **Resources Optimal Utilization**
- **Bio-Technologies**

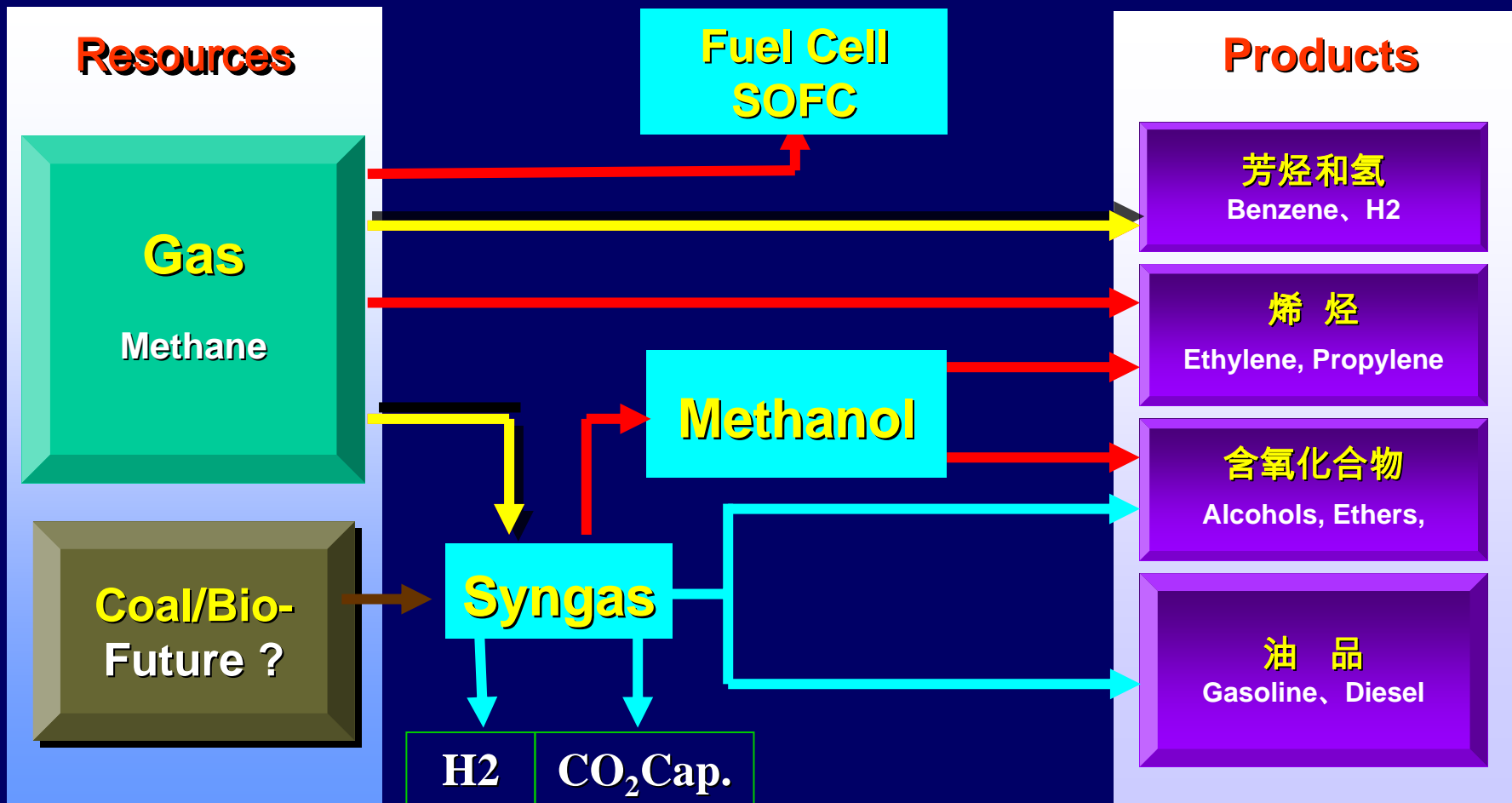
Energy Researches in DICP

- **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

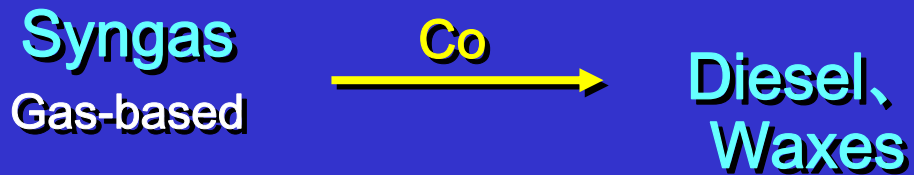
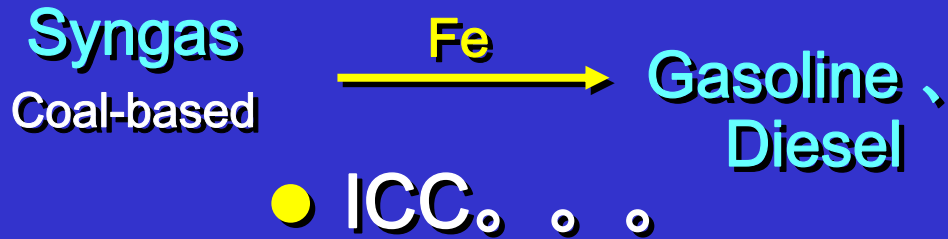
Key Techniques to Polygeneration



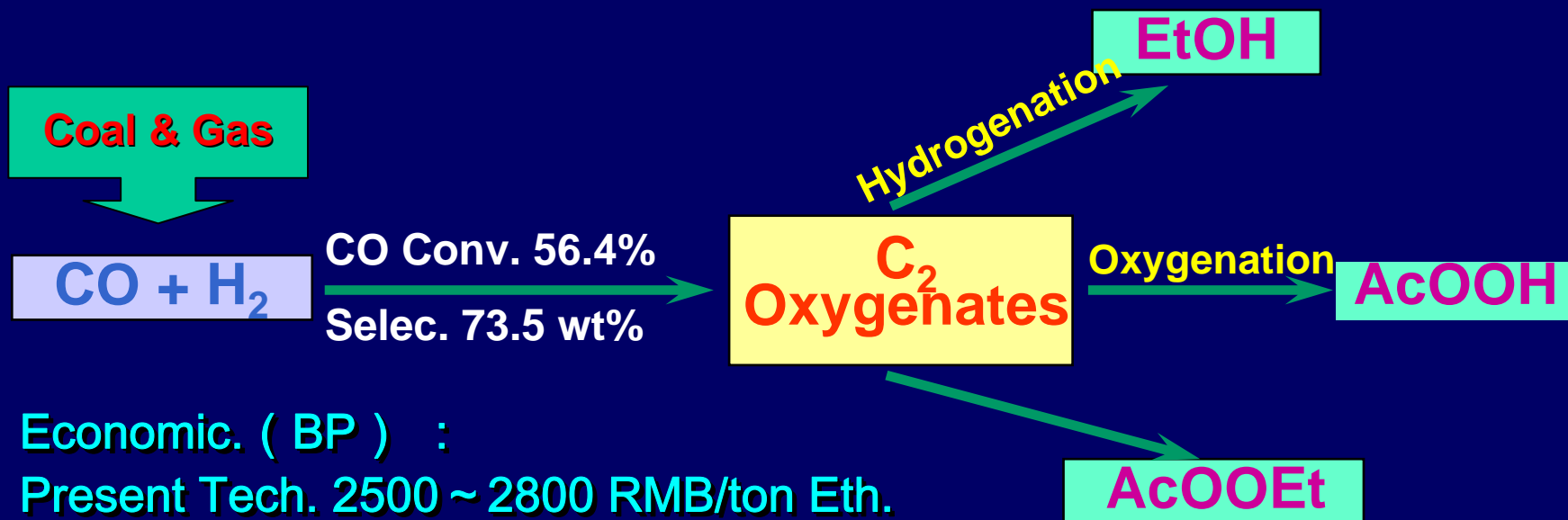
Utilization of Natural Gas & Coal



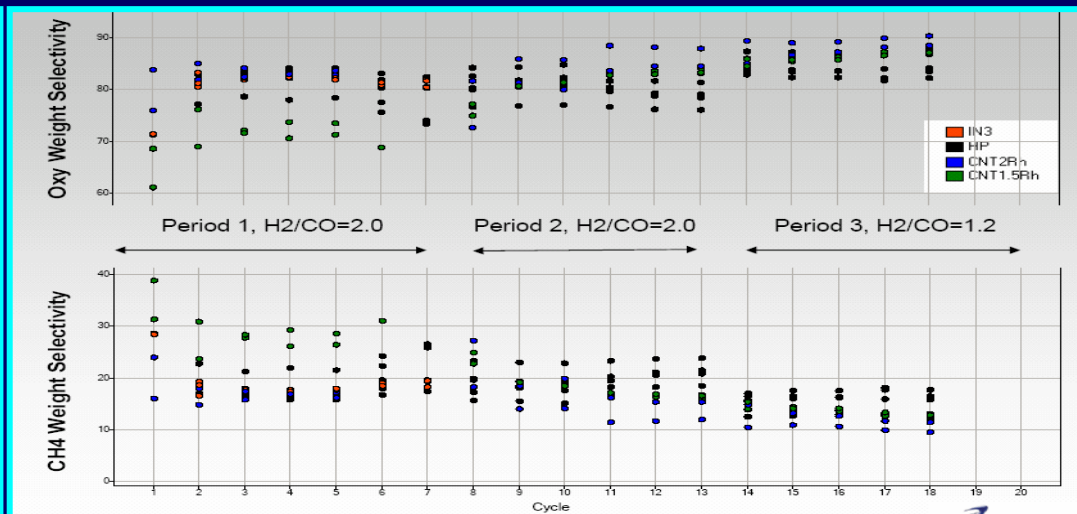
Gas to Liquid (GTL)



C2 Oxygenates from Syngas

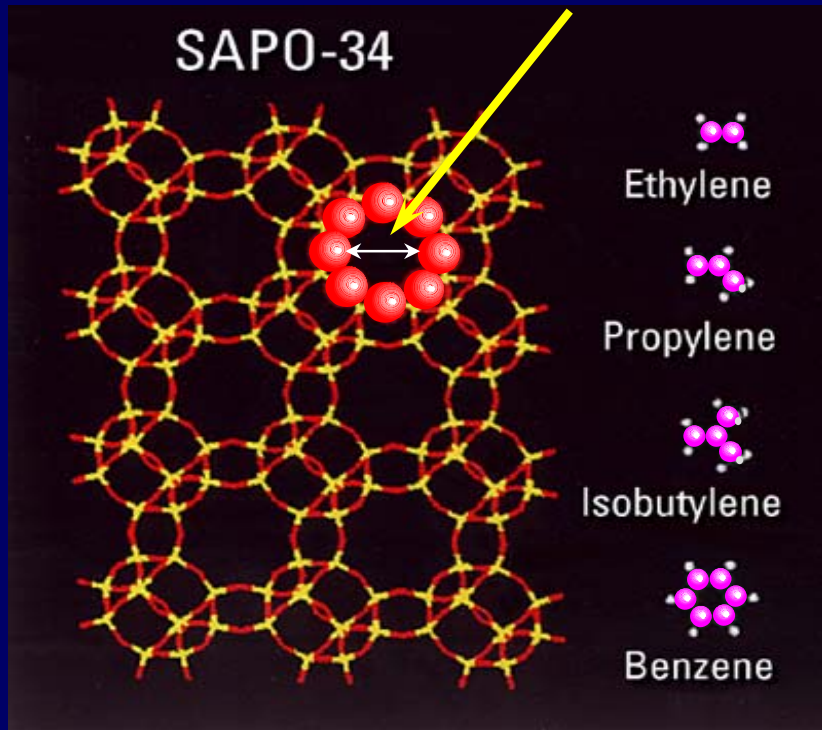


Economic. (BP) :
Present Tech. 2500 ~ 2800 RMB/ton Eth.

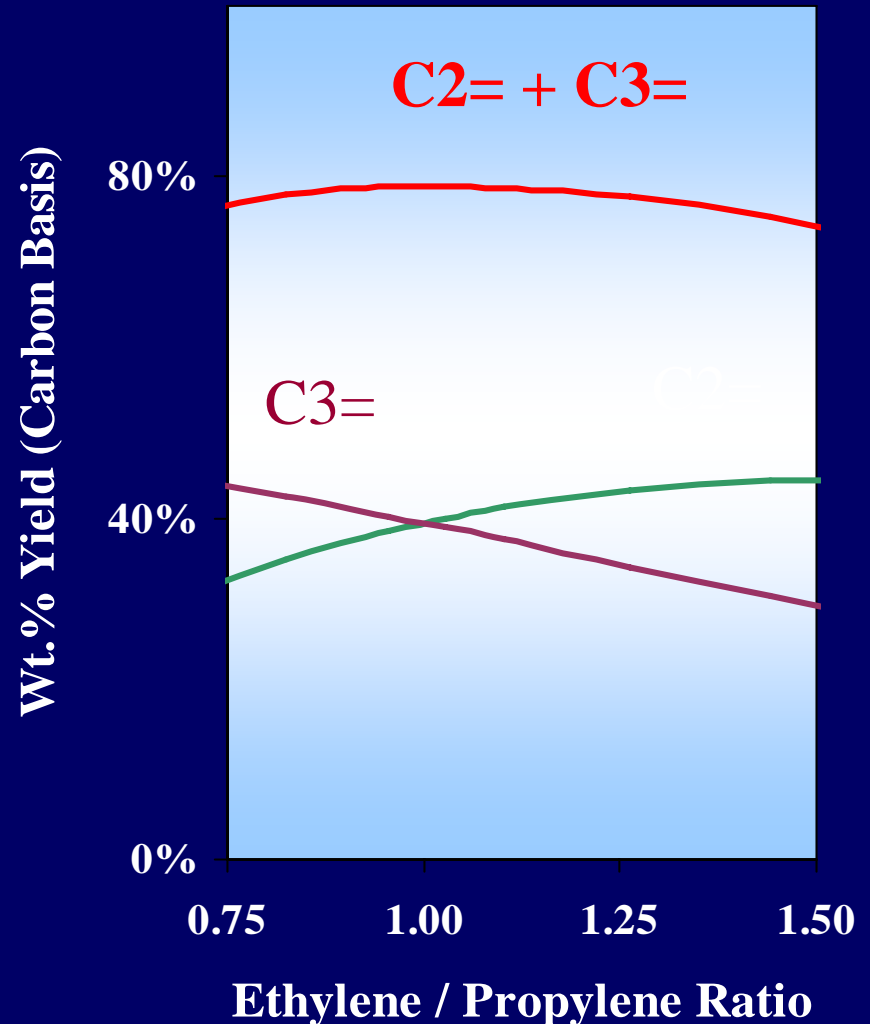


Methanol to Olefins (MTO)

3.8 Angstroms

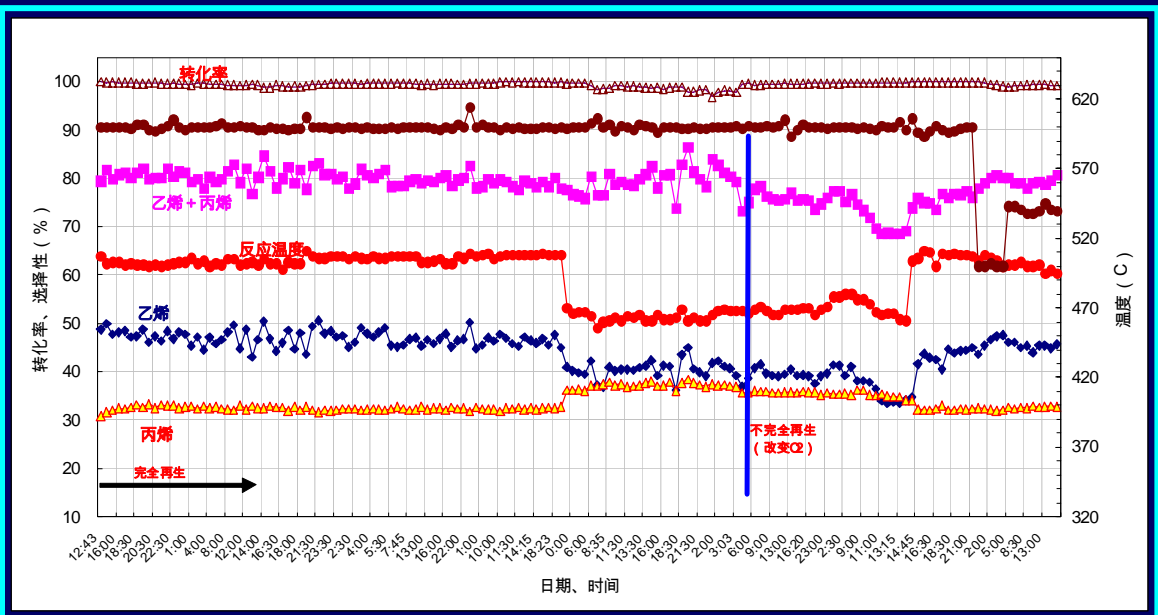


The unique pore size allows the selective conversion to olefins and excludes heavier compounds



Pilot and Demo of the MTO process

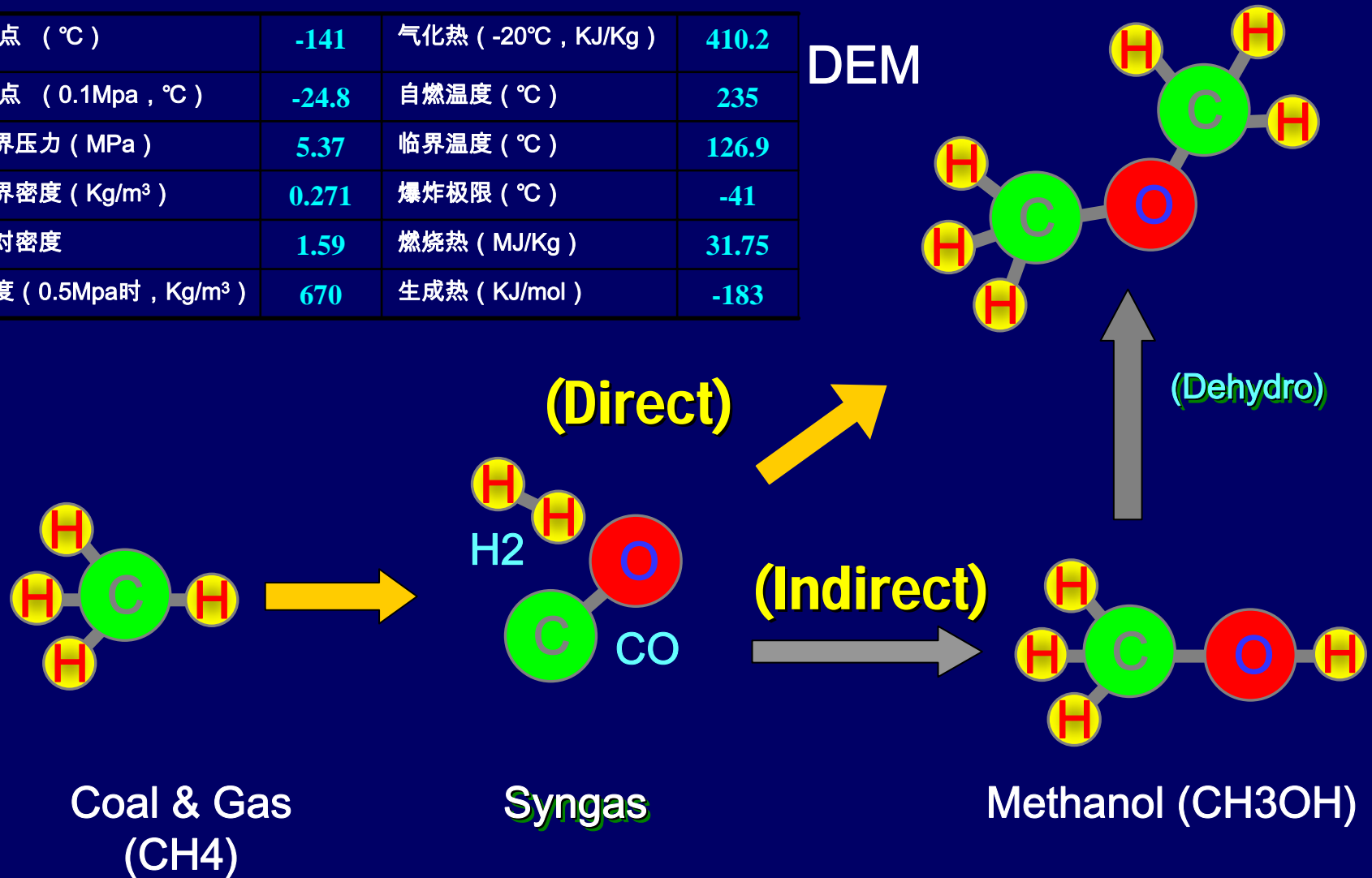
- Shanxi Coal Company (86million RMB)
- Sinopec Leyang Eng. Comp. (Tech Design)
- DICP (Catalyst & Process)



Dimethyl Ether (DME) and its Manufacture

熔点 (°C)	-141	气化热 (-20°C , KJ/Kg)	410.2
沸点 (0.1Mpa , °C)	-24.8	自燃温度 (°C)	235
临界压力 (MPa)	5.37	临界温度 (°C)	126.9
临界密度 (Kg/m ³)	0.271	爆炸极限 (°C)	-41
相对密度	1.59	燃烧热 (MJ/Kg)	31.75
密度 (0.5Mpa时 , Kg/m ³)	670	生成热 (KJ/mol)	-183

DEM



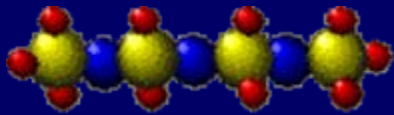
“Poly-DME-DMM” _ Diesel Substitution



DME



Dimethoxymethane
(DMM)



Dimethyldioxymethylene
(DMM₂)



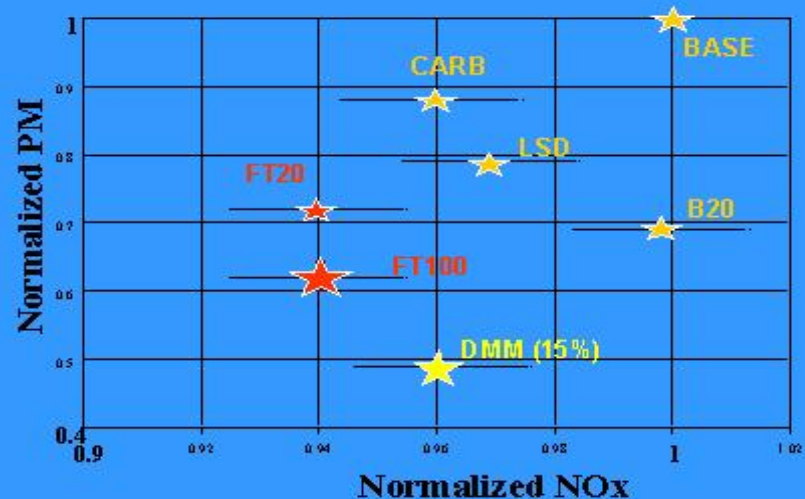
Poly-Dimethoxymethane
(DMM_x)

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

	DMM	DMM ₂	DMM ₃₋₈
BP, °F	42	105	152-315
Flash Pt., °F	0	<24	65
Cetane No.	28	41	76

PM and NOx Emissions of 7 test fuels



Source: DOE/SWRL

Development of PE Fuel Cell



FUEL CELL ENGINE



2000

30KWH2/O2



2002

75KWH2/Air



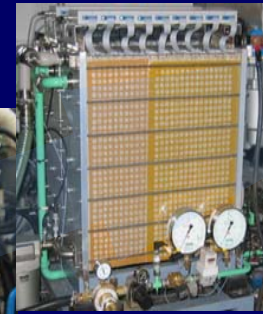
2003.8

90KWH2/Air



2003.10

100KWH2/Air



2003.12

100KWH2/Air

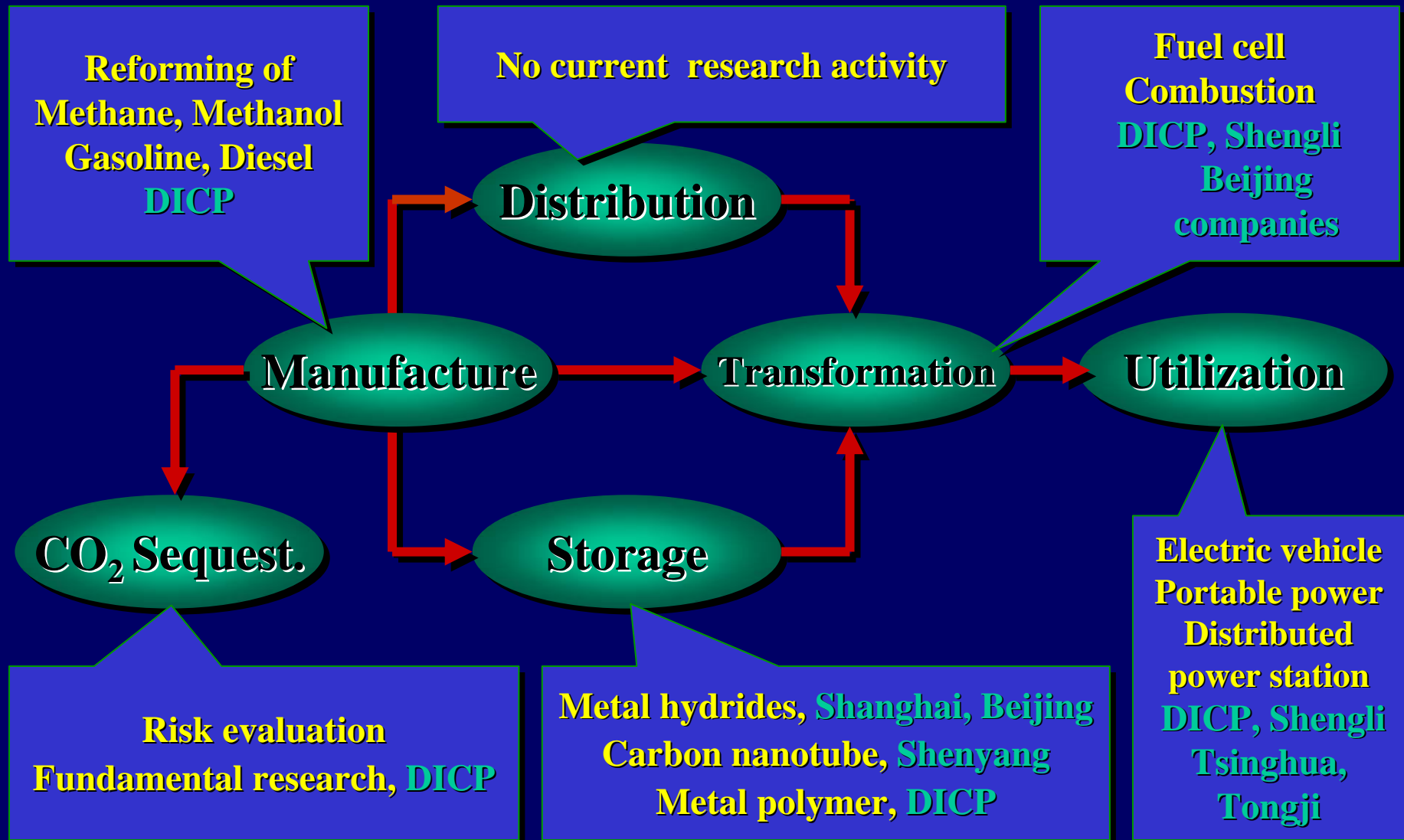


2004

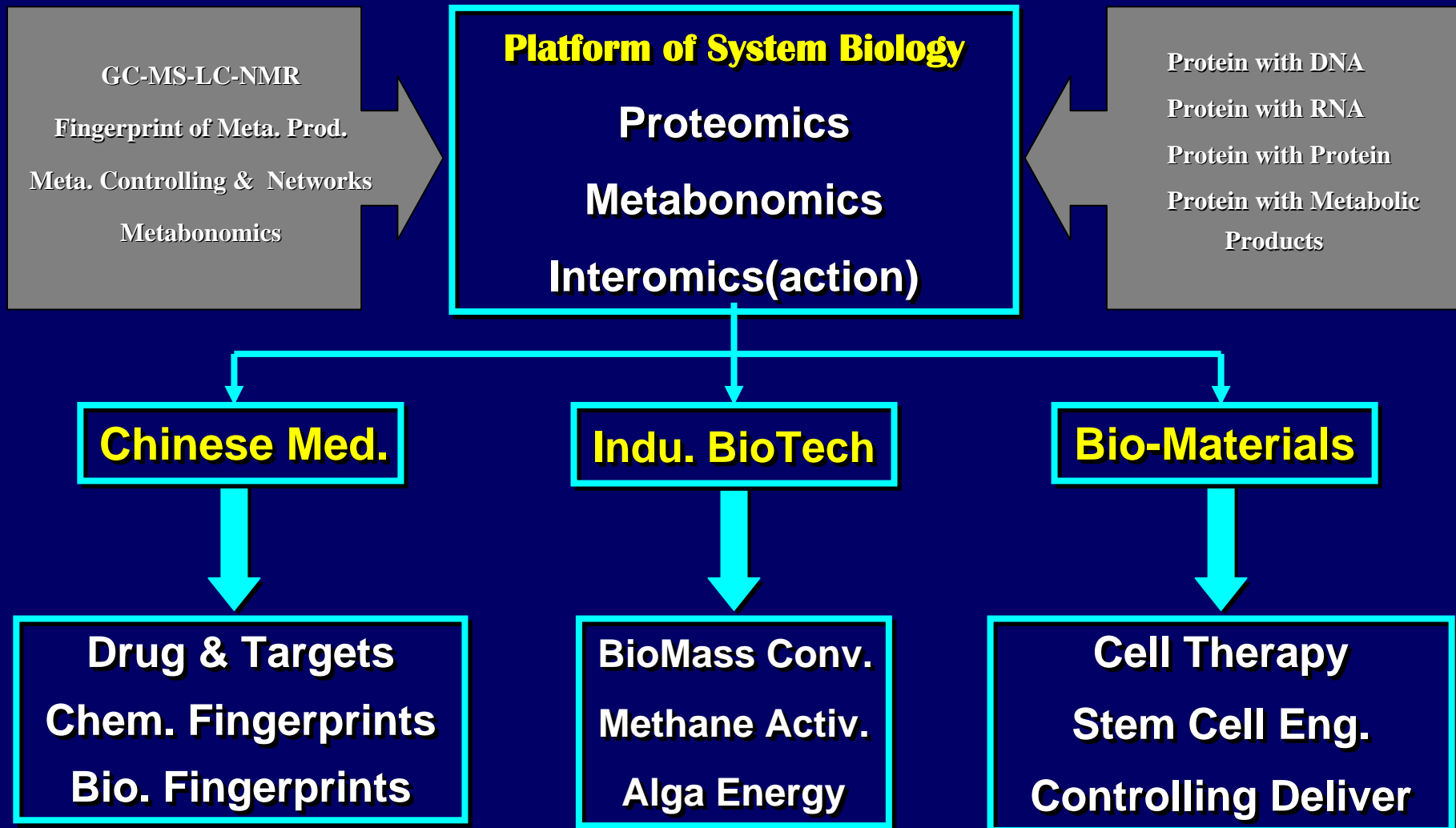
150kwH2/Air



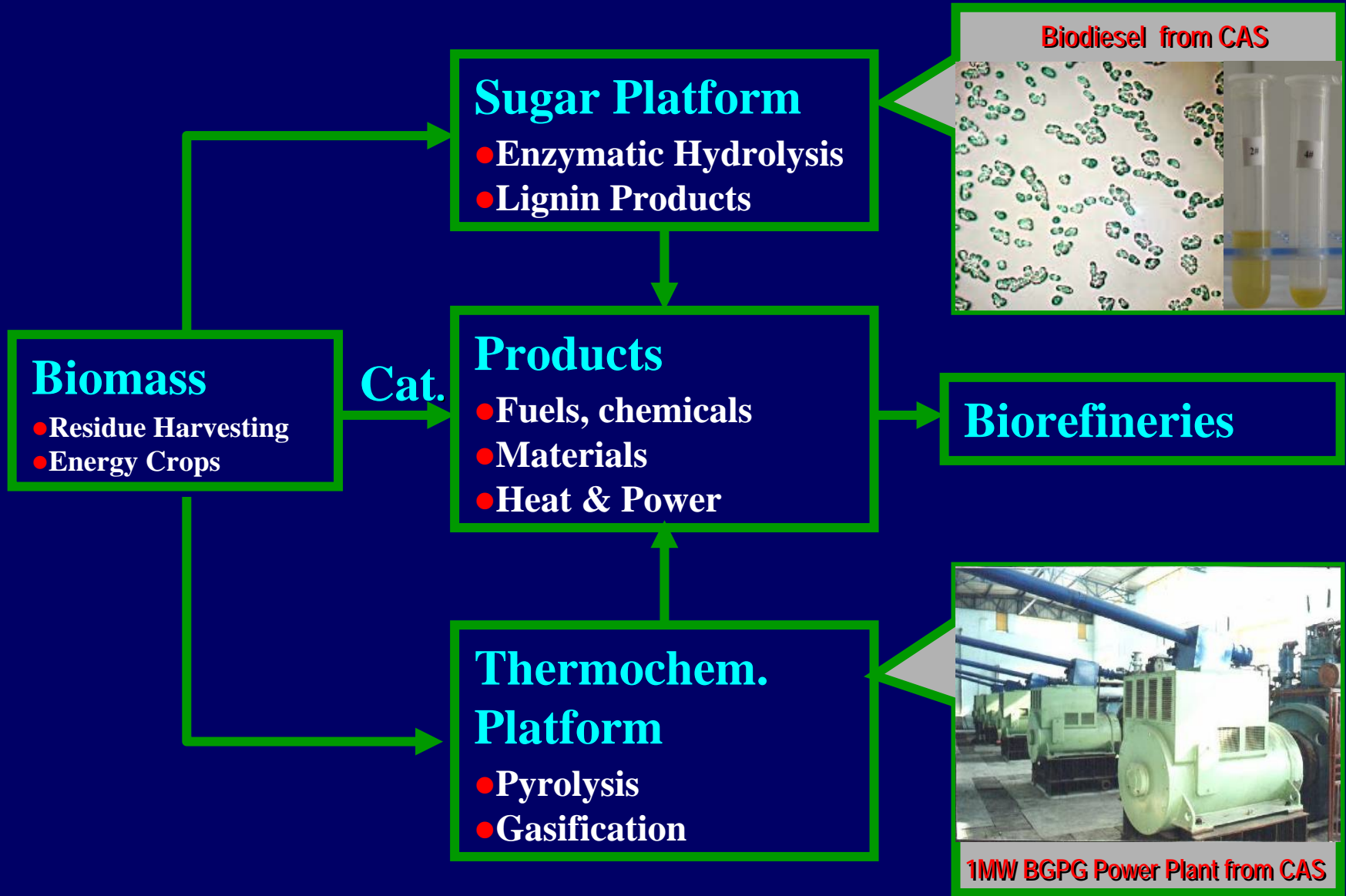
Hydrogen Related Researches in DICP



Strategy of Bio-Technology in DICP



Biomass Utilization at DICP



Dalian National Lab of Clean Energy

Oil & Gas Conver.

National Eng. Cent.

Sinopec

Fuel Cell & hydrogen

State Key Lab.

PetroChina

Bio-Energy

Research Cent of DICP

Gov. Program

Solar Energy

Foundation

Energy Environment

Enterprises

Energy Fundament

Strategic & evalu.



Energy Demo
SINOPEC, BP, Gov.

International Co.
BP, CNRS, BASF

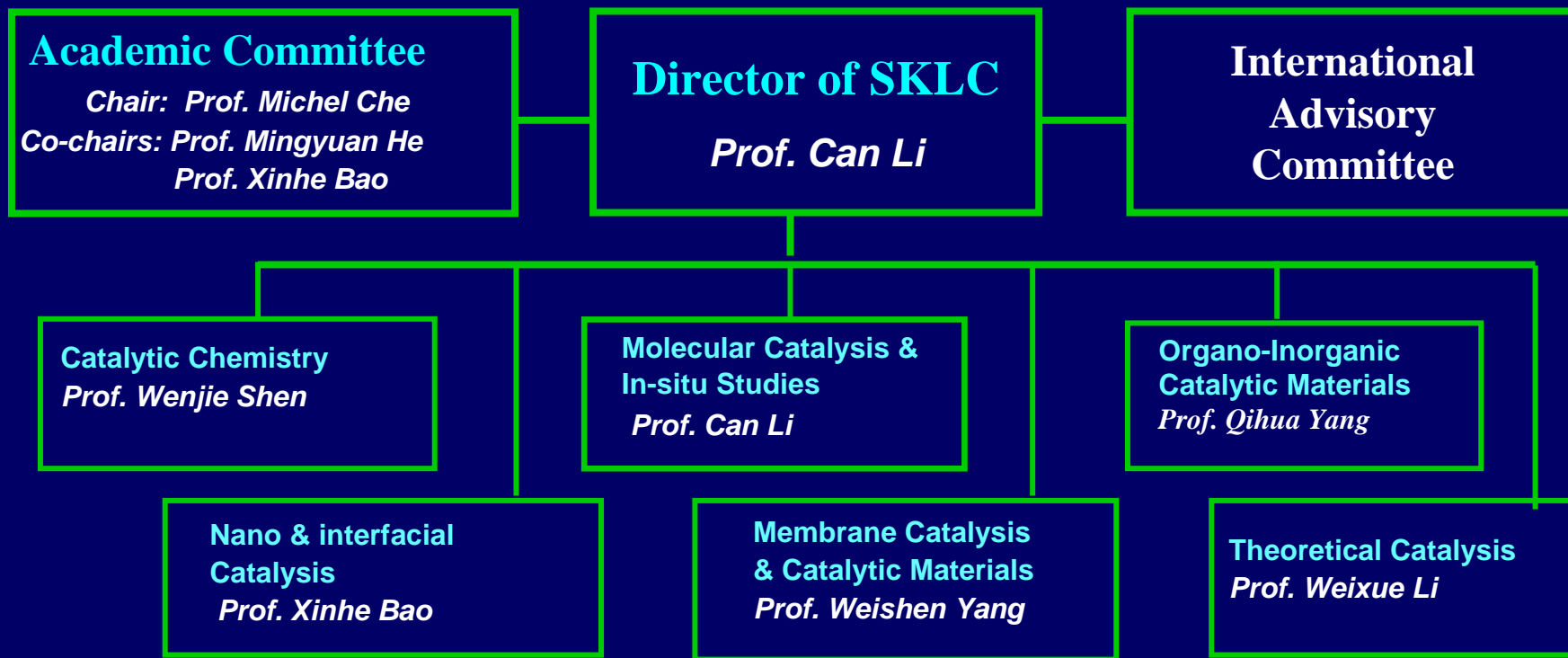
Catalysis researches at DICP

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)



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

NO_x 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**

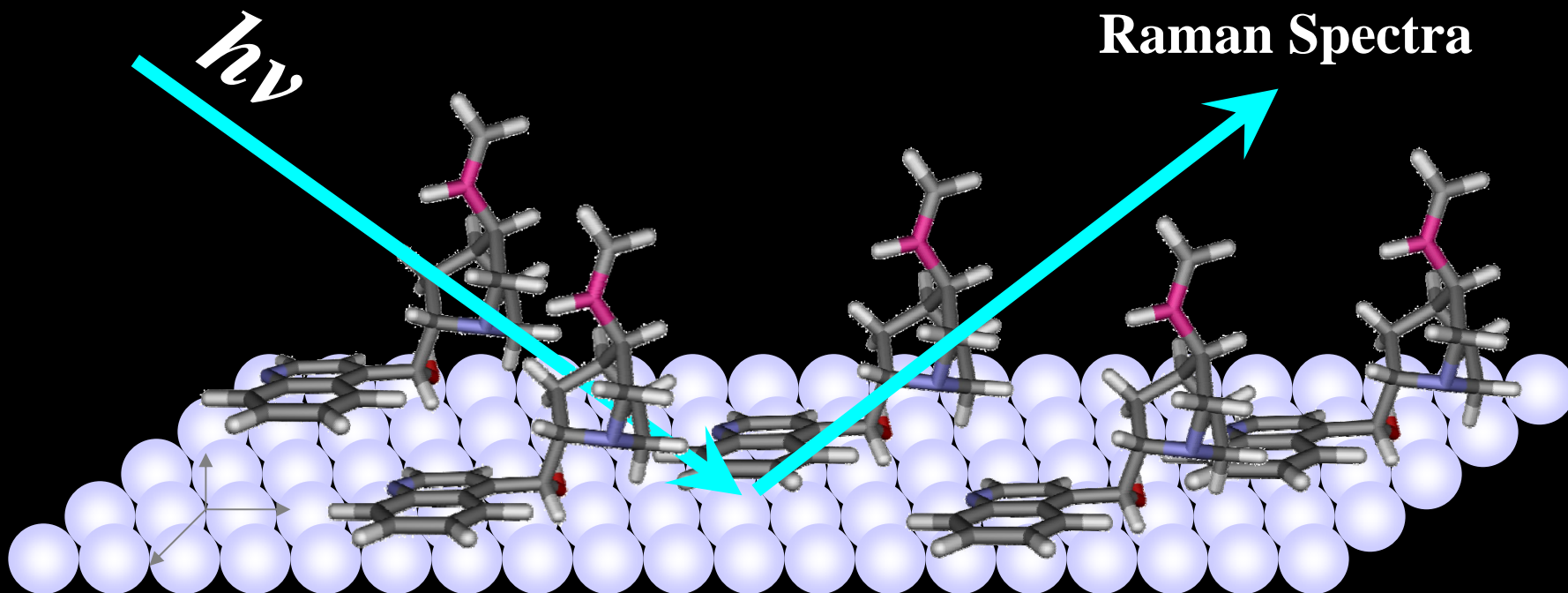
XRD, SEM, TEM, EDX, BET, ...

- **Atomic, molecular and nano scale**

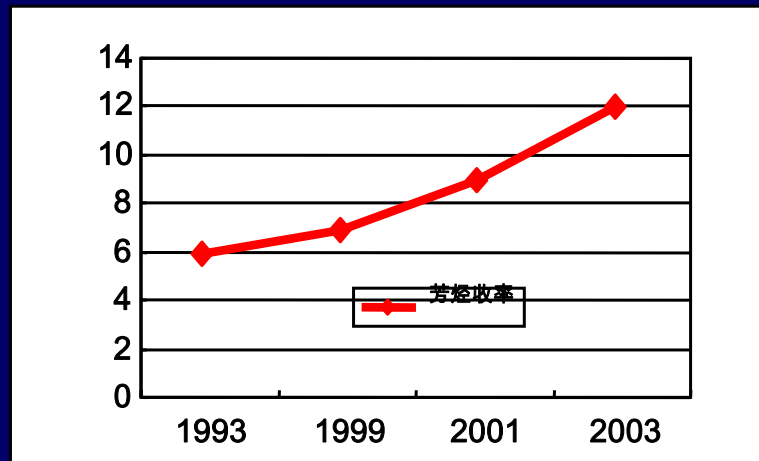
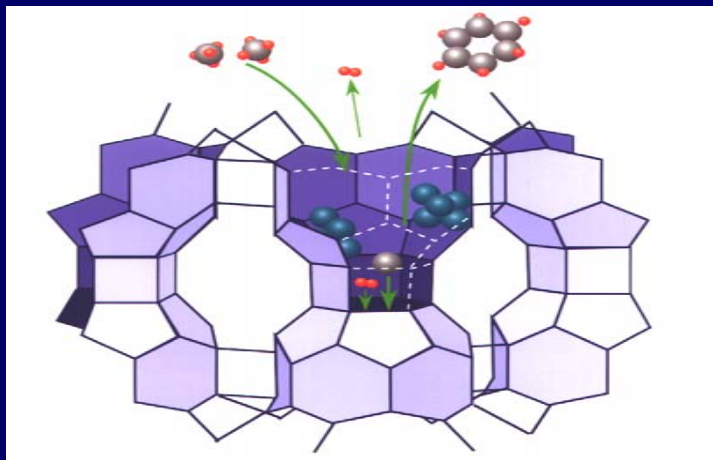
Multi Nano-Probe, HREELS, XPS, AES, LEED,

Achievements: Example 1

UV Resonance Raman Spectroscopic Studies on Catalysis

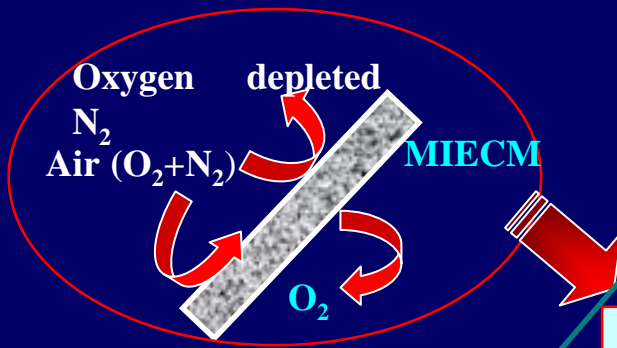


Non-oxidative Aromatization of Methane

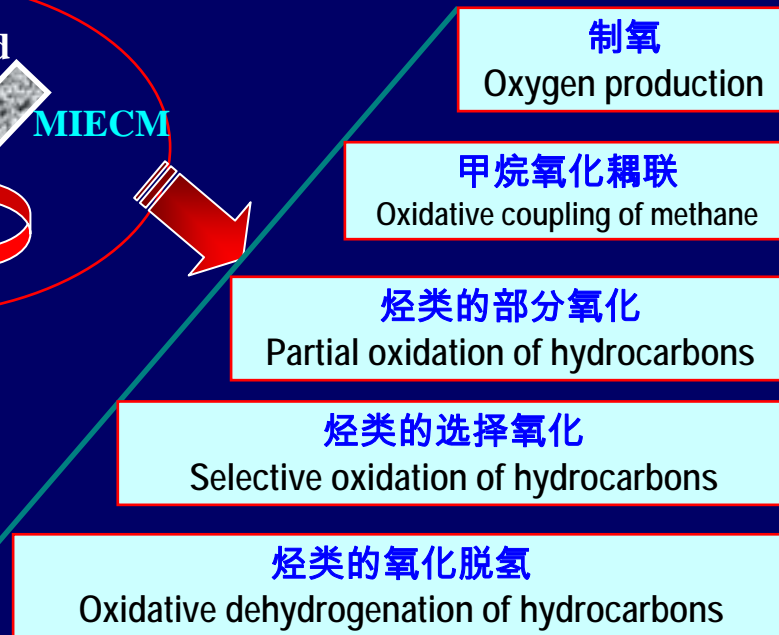


Achievements: Example 3

Applications of Mixed Ion & Electron Conductivity Oxygen Permeable Membrane



Dense ceramic membrane with mixed oxygen ionic and electronic conductivity



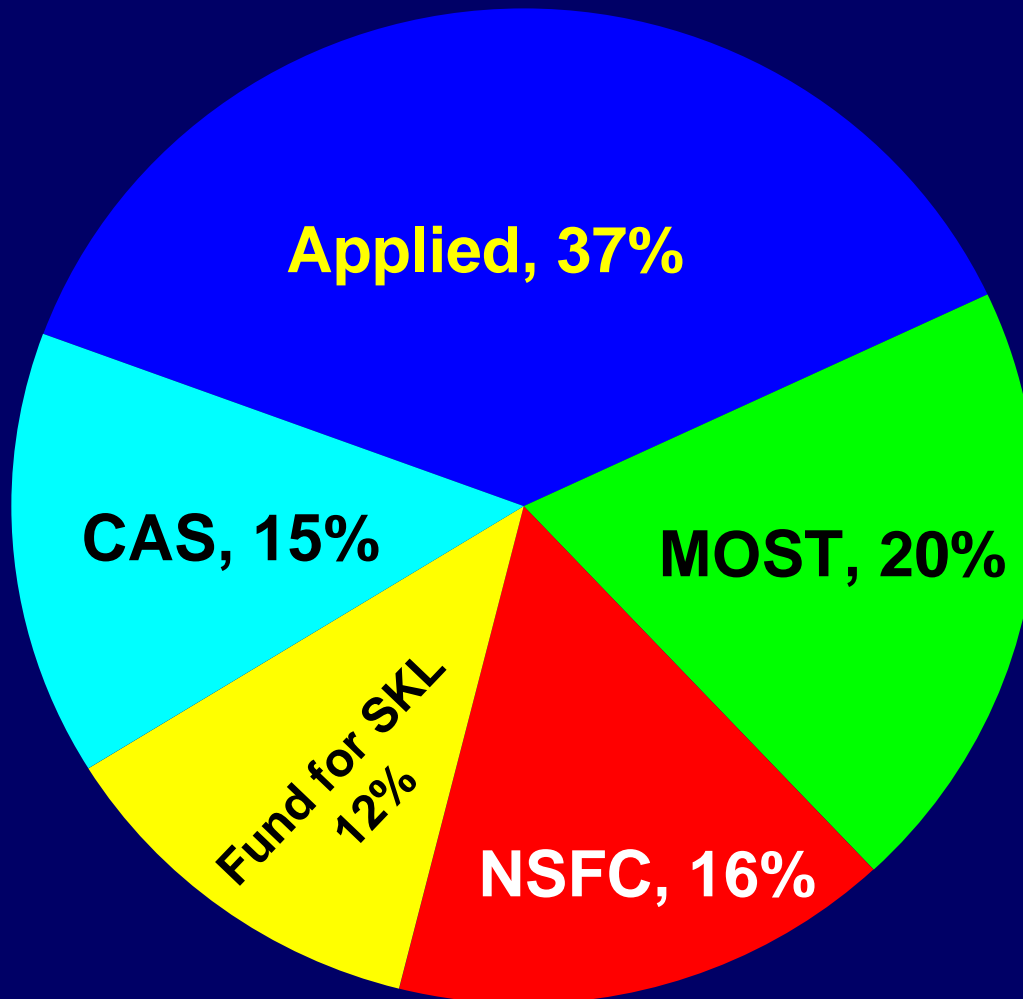
Oxygen Production:

- 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

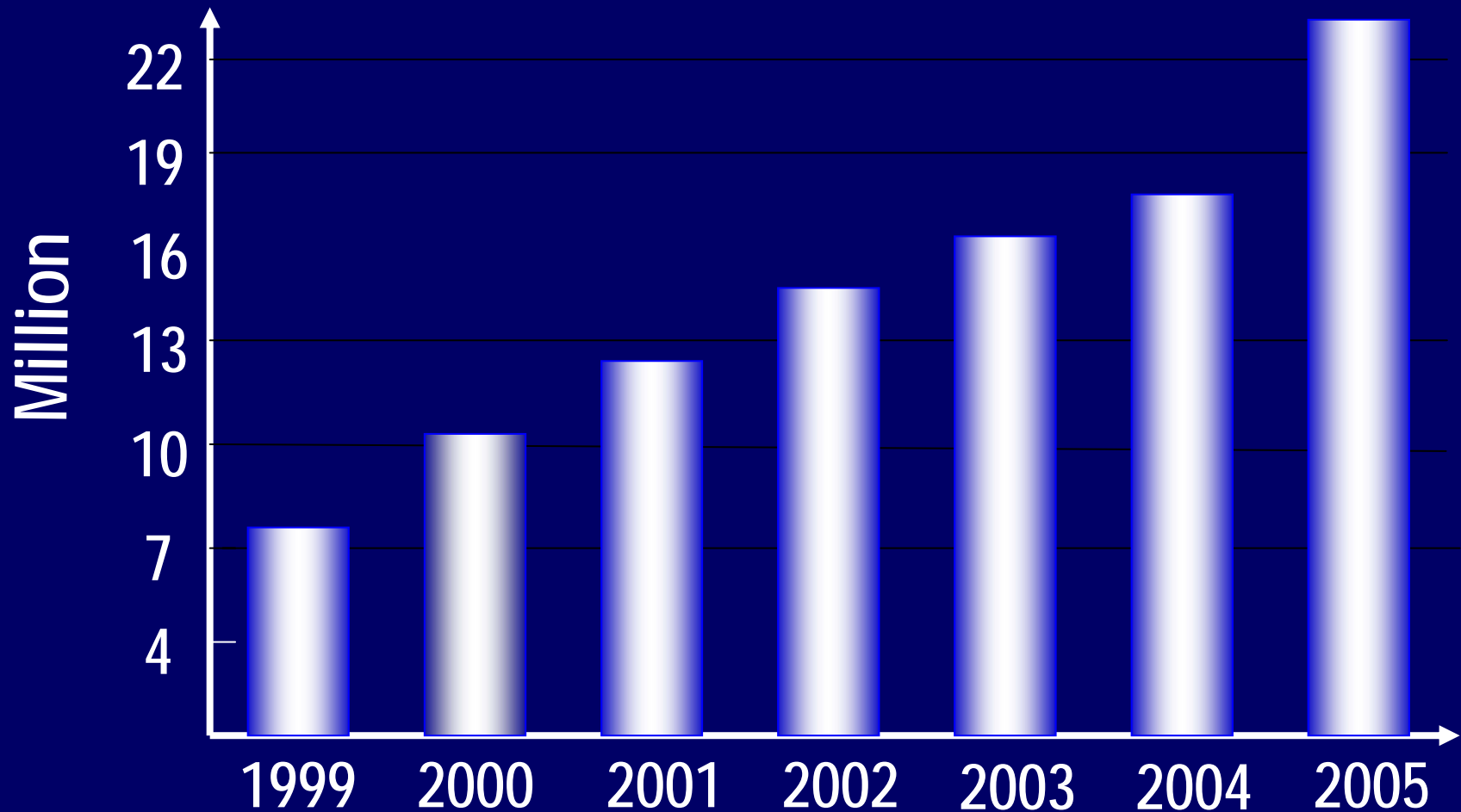
Composition of the Research Projects



Applied, 37%
Fundamental, ~ 63%

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

Budgets for Research in past years



Researches 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

Joint Projects

Domestic and overseas
Enterprises



Contract Researches

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-Samsung 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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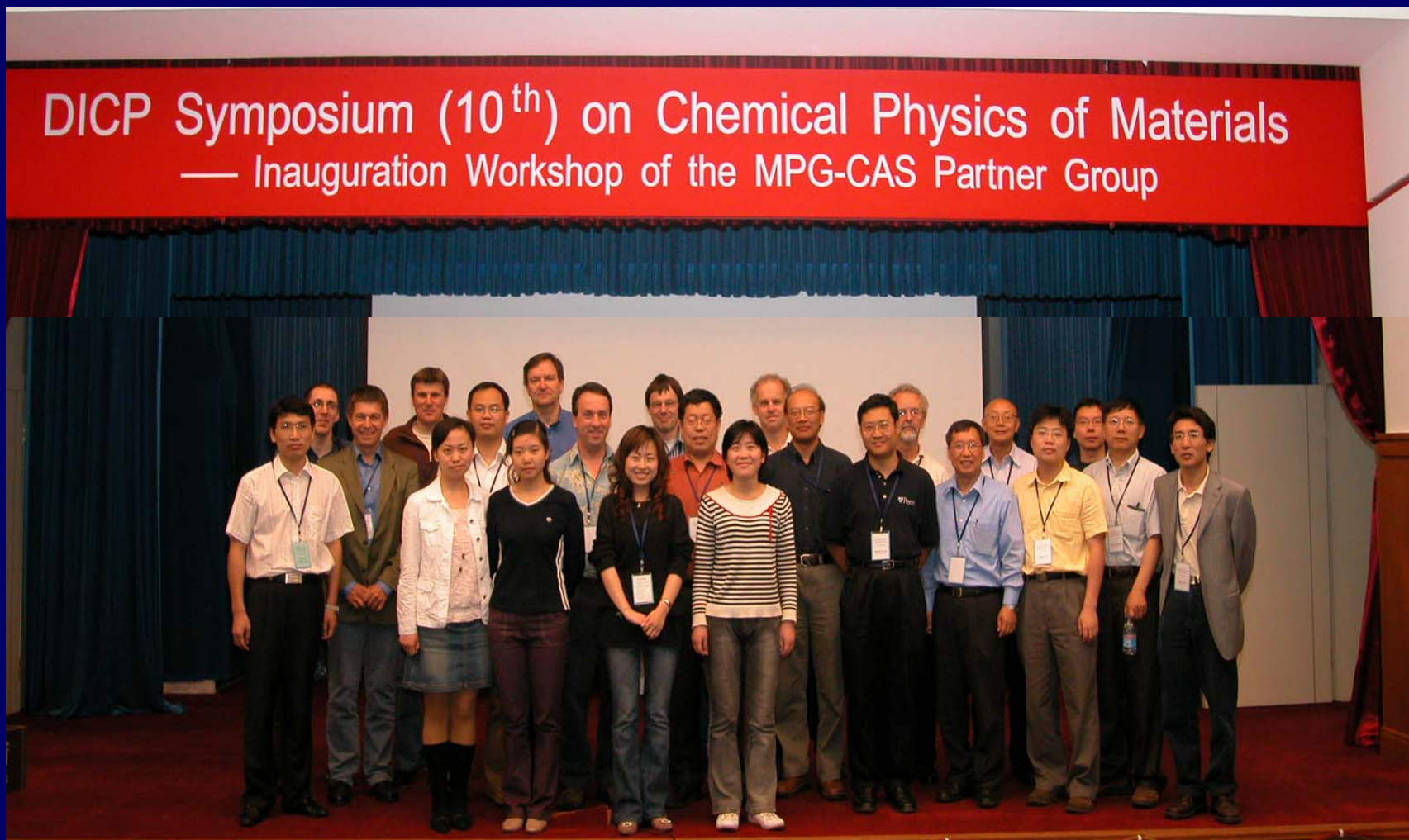
science crossing borders...

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**

DICP Symposium

DICP Symposium (10th) on Chemical Physics of Materials
— Inauguration Workshop of the MPG-CAS Partner Group



Thank for Attention



Welcome to DICP