

## Thursday, March 17, 2011

09:30~10:15	Registration
10:15~10:30	Opening Remarks 吳萬益 校長, 江國寧 主任
<b>Chair</b>	<b>江國寧 主任 國家高速與網路計算中心</b>
10:30~11:20	林明璋 院士 Why Ab Initio Quantum Simulation is Useful to Chemists and Materials Scientists?
11:20~12:10	劉梅林 傑出教授 Understanding the Surface and Interfaces in Fuel Cells: Modeling, Simulation, <i>in Situ</i> Characterization
12:10~14:30	Lunch & Poster exhibition
<b>Chair</b>	<b>靳宗政 主任 中國文化大學化學系</b>
14:30~15:00	林倫年 教授 Molecular Theory of Sum Frequency Generation Spectroscopy
15:00~15:30	鄭原忠 教授 Efficient Simulation of Two-Dimensional Electronic Spectroscopy: On Structural and Energetic Information of Multichromophoric Systems
15:30~16:00	包淳偉 教授 Nanoscale Morphology of Bulk Heterojunction Organic Photovoltaic Cells from Multiscale Molecular Simulations
16:00~16:30	Coffee Break
<b>Chair</b>	<b>梁贊全 主任 中正大學物理系兼通識教育中心</b>
16:30~17:00	朱訓鵬 教授 Finding the lowest-energy nanoparticle and nanowire structures by simulated annealing basin-hopping method
17:00~17:30	郭哲來 研究員 Exploring the structure of H-bonded Clusters via Multi-model Methods
17:30~18:00	關肇正 研究員 Electronic Transport in Alkanedithiol Single-Molecule Junctions
18:00~20:00	Banquet

**Friday, March 18, 2011**

09:00~10:00	Registration
<b>Chair</b>	<b>何嘉仁 教授 臺灣師範大學化學系</b>
10:00~10:30	江志強 教授 Theoretical Study of Molecular Engineering in Conjugated Polymers with Intramolecular Donor-Acceptor Interactions
10:30~11:00	吳宗信 教授 Parallel Fluid Modeling and Gas Flow Simulation for General Gas-Discharge Applications
<b>Chair</b>	<b>盧建銘 副組長 國家高速與網路計算中心</b>
11:00~11:30	陳俊杉 教授 Multiscale Modeling of Microcantilever Biosensors
11:30~12:00	王伯昌 教授 A Theoretical Investigation in Carbon, Boron-Nitride Nanotubes and Graphene Nanoribbons
12:00~14:00	Lunch & Poster exhibition
<b>Chair</b>	<b>楊志開 教授 政治大學應用物理研究所</b>
14:00~14:30	王禎翰 教授 Mechanism of Ethanol Reforming on Close-Packed Transition Metals: Oxidation, Dehydration and Decomposition
14:30~15:00	李豐穎 教授 Docking study of the precursor peptide of matoparan onto its putative processing enzyme, dipeptidyl peptidase IV: a revisit to molecular ticketing
15:00~15:30	Coffee Break
<b>Chair</b>	<b>洪祐明 教授 中國文化大學化學系</b>
15:30~16:00	孫英傑 教授 Computer-aided Drug Design: Anti-cancer Studies
16:00~16:30	蔡明剛 教授 Theoretical Perspective in the Anodic Reaction of Water Splitting by Molecular Ruthenium Catalysts
16:30~17:00	Poster Contest Prize & Closing