2015 6/16 Tuesday

08:00~08:45	REGISTRATION		
08:45~09:00	OPENING: Mei-Yin Chou, IAMS DIRECTOR (IB - 101)		
09:00~09:45	PLENARY 1: John S. Tse		
09:45~10:00	COFFEE BREAK		
	IB - 101	IB - 201	IB - 202
10:00~12:00	Section 1A	Section 1B	Section 1C
12:00~13:30	GROUP PHOTO + LUNCH		
13:30~15:00	Section 2A	Section 2B	Section 2C
15:00~15:30	COFFEE BREAK		
15:30~16:30	Section 3A	Section 3B	Section 3C
16:30~17:00	COFFEE BREAK		
17:00~18:30		Section PA	Section PB
18:30~19:00	Dinner/Poster Prepare (12F)		
19:00~20:00	POSTER SESSION		

2015 6/17 Wednesday

08:30~09:00	REGISTRATION		
09:00~09:45	PLENARY 2: Peijun Hu (IB - 101)		
09:45~10:00	COFFEE BREAK		
	IB - 101	IB - 201	IB - 202
10:00~12:00	Section 4A	Section 4B	Section 4C
12:00~13:30	LUNCH		
13:30~15:00	Section 5A	Section 5B	Section 5C
15:00~15:30	COFFEE BREAK		
15:30~17:40	Section 6A	Section 6B	Section 6C
17:40~18:30	Goto Banquet		
BANQUET			

2015 6/18 Thursday

08:30~09:00	REGISTRATION		
09:00~09:45	PLENARY 3: Puru Jena (IB - 101)		
09:45~10:00	COFFEE BREAK		
	IB - 101	IB - 201	IB - 202
10:00~11:30	Section 7A	Section 7B	Section 7C
11:40~12:30	SPECIAL TALK by Yoshiyuki Kawazoe + CLOSING/AWARD (IB - 101)		
LUNCH			

2015 6/16 Tuesday

08:00~08:45	**REGISTRATION**

PLENARY 1, IB – 101

08:45~09:00	OPENING: Mei-Yin Chou, IAMS DIRECTOR
09:00~09:45	**John S. Tse** Chair: Mei-Yin Chou *Order out of Disorder: Pressure-induced Devitrification of Glasses*

Section 1A, IB – 101 (Chair: Khian-Hooi Chew)

10:00~10:30	**Rauzah Hashim** *Structural and Dynamical Properties of Anhydrous Bilayers from Sugar Based Lipids: An Atomistic Simulation Study*
10:30~11:00	**Vannajan Sanghiran Lee** *Theoretical antiviral protein design targeting HIV-1 capsid through molecular dynamics simulations*
11:00~11:30	**Ming-Hsien Lee** *Lone Pair Electrons and Second Harmonic Generation in Oxide Crystals: A DFT Study*
11:30~12:00	**Lam K. Huynh** *A Computational Study on the Adsorption Configurations and Reactions of SiH_X(X=1-4) on Clean and H-covered Si(100) Surfaces*

Section 1B, IB – 201 (Chair: Jer-Lai Kuo)

10:00~10:30	**Vladimir Belosludov** *Theoretical Study of the Boson Peak Origin in the Low Density Amorphous Ice*
10:30~11:00	**Toshiaki Iitaka** *X-ray Raman Spectroscopy Measurement for Detecting Pressure-induced Dissociation of Water Molecules in Ice VII*
11:00~11:30	**Chin-Lung Kuo** *Atomic-Scale Modeling of the Mechanical and Dielectric Properties of the Ultra-Low-k Nanoporous Silicate Glasses*
11:30~12:00	**Ying Chen** *Elastic Properties of Dilute Si in Fe-Si Alloy and Effect of Ni-Doping: An Integrated Study Based on First-Principles*

2015 6/16 Tuesday

Section 1C, IB – 202 (Chair: Yu-Chang Chen)

10:00~ 10:30	**Makusu Tsutsui** *Single-Molecule Sequencing Using Nanopores and Nanoelectrodes*
10:30~ 11:00	**Yu-Hui Tang** *Spin Torque Effect in Spin-Filter Based Magnetic Tunnel Junction*
11:00~ 11:30	**Chao-Cheng Kaun** *Spin-polarized Transport through Single-molecule Magnetic Junctions*
11:30~ 12:00	**Ilias Amanatidis** *Local Heating and Cooling criterion in Nanoscale Systems*

Section 2A, IB – 101 (Chair: Chao-Ping Hsu)

13:30~ 14:00	**Hui-Hsu Gavin Tsai** *Computational Investigation of Electron Injection of Squaraine Dye-Sensitized Solar Cells*
14:00~ 14:30	**Jiann T'suen Lin** *Metal-Free Sensitizers for Dye-Sensitized Solar Cells: Structure/Performance Correlation*
14:30~ 15:00	**Yu-Tai Tao** *Polyfused Aromatics as Charge Transport Materials in Field-Effect Transistor Applications: A Structure-Property Correlation Study*

Section 2B, IB – 201 (Chair: Gour Prasad Das)

13:30~ 14:00	**Guang-Yu Guo** *Ab Initio Calculation of Plasmon Excitations in Graphene and Nonlinear Optical Properties of Transition Metal Dichalcogenide Monolayers*
14:00~ 14:30	**Jisoon Ihm** *Magnetic ordering on edges of topological insulators*
14:30~ 15:00	**Balazs Hetényi** *The Topology of Ideal Conduction*

Section 2C, IB – 202 (Chair: Duc Nguyen-Manhm)

13:30~ 14:00	**Xin-Gao Gong** *Inverse Design and Computational Studies of Novel Solar Energy Materials*
14:00~ 14:30	**Yu-Chang Chen** *Thermoelectric properties in atomic/molecular junctions from first principles*
14:30~ 15:00	**Patrick Sit** *First Principles Study of Redox Reactions for Energy Storage and Conversion*

2015 6/16 Tuesday

	Section 3A, IB – 101 (Chair: Chao-Ping Hsu)
15:30~ 15:50	**Hockseng Nguan** *Dynamics and Anomalous diffusions in the liquid crystals inverse hexagonal phase: a molecular dynamics simulation study*
15:50~ 16:10	**Yun-Wen Chen** *Theoretical Investigation of Using Silsesquioxane Frameworks for Hydrogen Storage System*
16:10~ 16:30	**Arkapol Saengdeejing** *First-principles study of stability of Cu in the Nd-rich and Nd Oxide phases of Nd-Fe-B permanent magnet*

	Section 3B, IB – 201 (Chair: Ming-Kang Tsai)
15:30~ 15:50	**Hirobumi Mineo** *Adiabatic treatment for vibrational predissociation of water dimers with channel interactions*
15:50~ 16:10	**Yu-Lin Yeh** *A Theoretical Investigation of Surface-enhanced Sum-Frequency Generation*
16:10~ 16:30	**Ermias Girma Leggesse** *New Conductive Imidazole-derived Salt for Lithium-ion Battery Electrolytes: a DFT study*

	Section 3C, IB – 202 (Chair: Kaito Takahashi)
15:30~ 15:50	**Tzu-Jen Lin** *Predicting New Phases of Solid Methanol*
15:50~ 16:10	**Yulia Yu. Bozhko** *Modeling of Composition and Formation Conditions of Double Hydrates of Tetrafluoromethane or Nitrous Oxide with methane*
16:10~ 16:30	**Santhanamoorthi Nachimuthu** *Enhanced Hydrogen Storage Performance of Boron-doped Graphene decorated by Ni-Ti-Mg atoms -A DFT study*

	Flash Talks (Chairs: Ming-Kang Tsai, Kaito Takahashi)
17:00~18:30	**Section PA at IB – 201; Section PB at IB – 202**
18:30~20:00	**POSTER SESSION and DINNER 12F**

2015 6/17 Wednesday

08:30~09:00	**REGISTRATION**

PLENARY 2, IB – 101

09:00~09:45	**Peijun Hu** Chair: Jyh-Chiang Jiang *Rational Catalyst Design in Heterogeneous Catalysis: Density Functional Theory Studies*

Section 4A, IB – 101 (Chair: Jyh-Chiang Jiang)

10:00~10:30	**Shang-Bin Liu** *A Novel Acidity Scale for Acidic Catalysts Based on ^{31}P NMR Chemical Shifts of Phosphine Oxide Probe Molecules*
10:30~11:00	**Aloysius Soon** *Non-conventional supports for single-atom nanocatalysts for the oxygen reduction reaction*
11:00~11:30	**Shawn D. Lin** *Metal-oxide interface for sustainable hydrogen production with ethanol steam reforming over Cu-NiO catalyst*
11:30~12:00	**Hsin-Tsung Chen** *CO Oxidation and C_2H_4 Epoxidation Catalyzed by a Gold Nanoparticle: : A Computational Study*

Section 4B, IB – 201 (Chair: Chih-Kai Yang)

10:00~10:30	**Qiang Sun** *Phase Stability of Dichalcogenide Monolayers*
10:30~11:00	**Hongming Weng** *Quantum Spin Hall Effect in 2D Transition Metal Dichalcogenide Haeckelites*
11:00~11:30	**Viet Huy Nguyen** *Improving Performance of Electronic and Thermoelectric Graphene Devices by Strain Engineering*
11:30~12:00	**Hung-Chung Hsueh** *Dimensionality Effects on Bound Excitons in Few-layer BN*

Section 4C, IB – 202 (Chair: John S. Tse)

10:00~10:30	**Duc Nguyen-Manhm** *Nano-defect clusters in irradiated materials: First-principles assessment and multi-scale modelling*
10:30~11:00	**Kwang-Ryeol Lee** *Multiscale Simulation Study of Structure and Electronic Properties of Oxidized Silicon Nanowire*
11:00~11:30	**Hiroshi Mizuseki** *Materials Design on Energy-related Materials by Multiscale Simulations*
11:30~12:00	**Koji Akai** *Study of electronic structures and thermoelectric properties on conjugated ethylenetetrathiolate metal polymers*

2015 6/17 Wednesday

Section 5A, IB – 101 (Chair: Xin-Gao Gong)

13:30~ 14:00	**Satoshi Watanabe** *First-Principles Study on Electric and Dielectric Properties of Metal-Oxide Heterostructures in Nanoscale Devices*
14:00~ 14:30	**Jian-Tao Wang** *Three-connected Networks of Si in Disilicides*
14:30~ 15:00	**Chee Kwan Gan** *Phononic Properties of Metal Chalcogenides Bi2S3 and Sb2S3: A First-Principles Study*

Section 5B, IB – 201 (Chair: Puru Jena)

13:30~ 14:00	**Qian Wang** *A Pentagon Based Carbon Sheet*
14:00~ 14:30	**Su Ying Quek** *Quantum-confinement and Structural Anisotropy result in Electrically-Tunable Dirac Cone in Few-layer Black Phosphorous – Importance of interlayer interactions beyond van der Waals*
14:30~ 15:00	**Chih-Kai Yang** *Graphene, Graphane, and Their Composites*

Section 5C, IB – 202 (Chair: Kwang-Ryeol Lee)

13:30~ 14:00	**Vijay Kumar** *$CsSn(X_xY_{1-x})3$ (X and Y = Cl, Br, and I) mixed perovskites for photovoltaics*
14:00~ 14:30	**Gang Lu** *Exciton Diffusion and Charge Separation in Organic Photovoltaics*
14:30~ 15:00	**Kahyun Hur** *Linking Experiment and Theory for 3D Networked Binary Metal Nanoparticle -Triblock Terpolymer Superstructures*

Section 6A, IB – 101 (Chair: Jyh-Chiang Jiang)

15:30~ 16:00	**Toyoko Imae** *Roles of Amine and Iron Oxide on Exfoliation of Graphite*
16:00~ 16:30	**Gour Prasad Das** *Electronic structure and Transport properties of Graphene Nanoribbons*
16:30~ 17:00	**Wei-Hung Chiang** *Atmospheric-pressure controllable synthesis of heteroatom-doped carbon nanomaterials and its applications for electrochemical energy storage and conversion*
17:00~ 17:20	**Shi-Hsin Lin** *Activation and Tuning of Two-dimensional Materials for Hydrogen Evolution Reaction*
17:20~ 17:40	**Sirichok Jungthawan** *Deformation behavior of strained single-layer BN, graphene, and silicene under pressurized blister test*

2015 6/17 Wednesday

Section 6B, IB – 201 (Chair: Vijay Kumar)

15:30~ 16:00	**Swapan K. Ghosh** *Energy Density Functional Approach to Designing Functional Materials for Energy Applications*
16:00~ 16:30	**Seungwu Han** *Automatizing Ab initio Calculations for High-throughput Screening*
16:30~ 17:00	**Jiraroj T-Thienprasert** *First-principles study of M defects (M = Bi and Al) in orthorhombic $PbZrO_3$*
17:00~ 17:20	**Katsumi Hagita** *Study of phonon DOS of Carbon crystals from nested K4 lattice to BC-8 structure*
17:20~ 17:40	**Chih-Kai Lin** *Nitrogen Dopants and Vacancy Defects in Graphene Nanoflakes: Theoretical Study of Size-Dependent Electronic Excitation Properties*

Section 6C, IB – 202 (Vladimir Belosludov)

15:30~ 16:00	**Manoj Harbola** *Excited-state energy functionals and ionization potential theorem*
16:00~ 16:30	**Jeng-Da Chai** *TAO-DFT and Its Applications to Zigzag Graphene Nanoribbons*
16:30~ 17:00	**Ryoji Sahara** *First principles study of electronic structures and stability in structural materials*
17:00~ 17:20	**Miao Miao Wu** *Photoelectron Spectroscopy and Theoretical Study of Platinum Halides PtX_n (X = F, Cl, Br, I; n = 2-4)*
17:20~ 17:40	**Cheng-chau Chiu** *Ru Catalyzed Hydrodeoxygenation of Aromatic Oxygenates Derived from Biomass*

2015 6/18 Thursday

08:30~09:00 **REGISTRATION**

PLENARY 3, IB – 101

09:00~09:45

Puru Jena Chair: Jer-Lai Kuo

Superhalogens – A Bridge between Complex Metal Hydrides and Li-ion Batteries

Section 7A, IB – 101 (Chair: Yoshiyuki Kawazoe)

10:00~10:30 **Yuan Chung Cheng**

Theory for Electronic Couplings and Dynamics of Singlet Fission in Oligoacene Dimers

10:30~11:00 **Elise Yu-Tzu Li**

Factors Governing Strong Spin-Orbit Coupling and Fast Intersystem Crossing in Luminescent Materials: A Theoretical Perspective

11:00~11:30 **Kaito Takahashi**

Tug of war between H_3O+ versus Ar/OH

Section 7B, IB – 201 (Chair: Qian Wang)

10:00~10:30 **Khian-Hooi Chew**

Charge Compensation Phenomena at Ferroelectric Interface

10:30~11:00 **Zhifeng Liu**

Designing Nano-Valves for the Storage of Hydrogen under High Pressure

11:00~11:30 **Yasuhiro Senda**

Atomic force microscopy simulation covering wide range time-scale

Section 7C, IB – 202 (Chair: Qiang Sun)

10:00~10:30 **Hieu Chi Dam**

Sparse Modeling for Materials Design

10:30~11:00 **Yansun Yao**

Computational Material Discovery using the HPC-Based ab initio Methods

11:00~11:30 **Jyh-Shing Lin**

Theoretical study of reaction dynamics for C-X dissociation of XH_2C-C≡$CH_{(ads)}$/X-C≡$CCH_{3(ads)}$ (X= I and Br) adsorbed on Ag(111) surface

Special Session, IB – 101

11:40~12:10

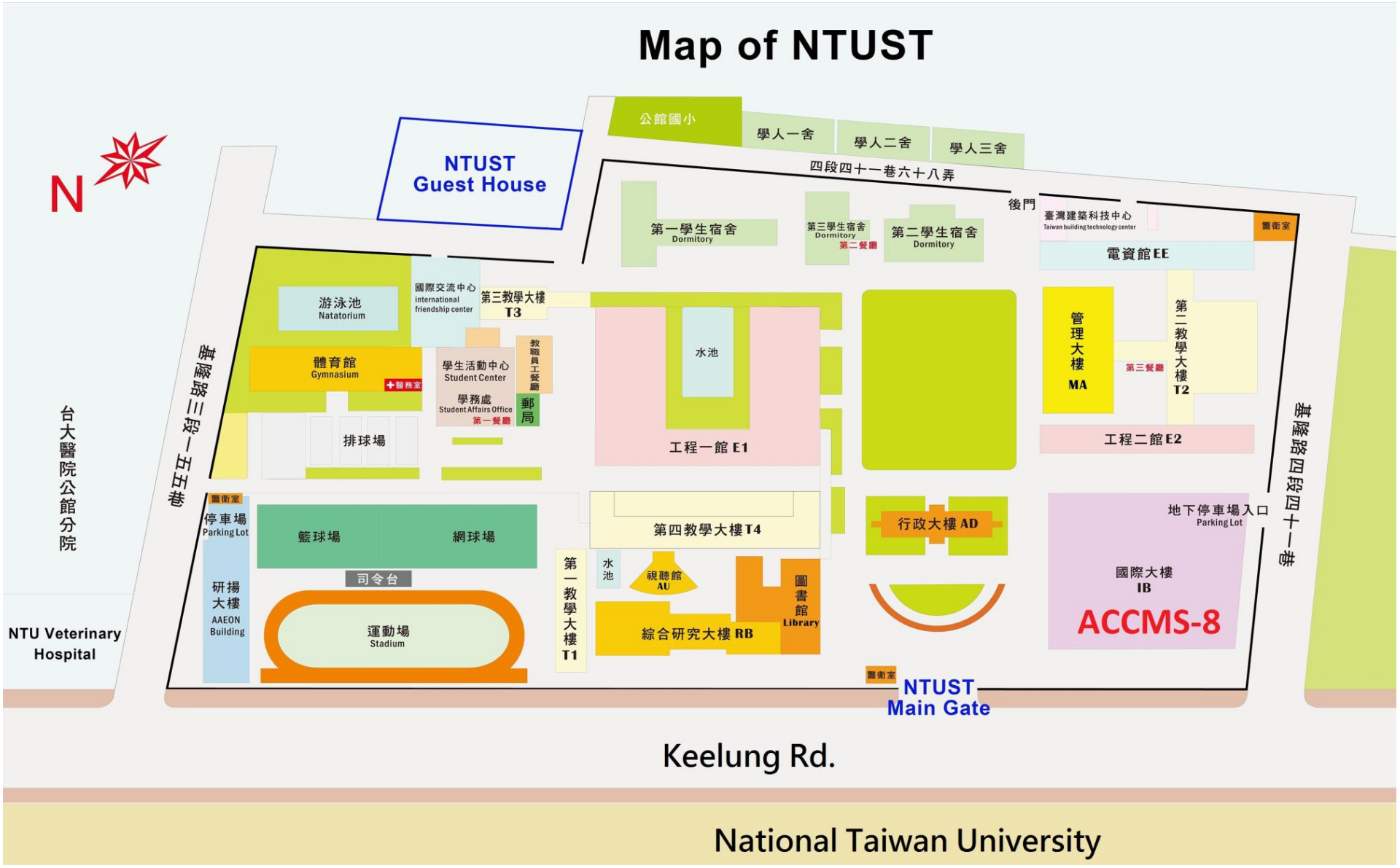
Yoshiyuki Kawazoe

Theoretical Study on Task Specific Ionic Liquid for Metal Extraction from Garbage Caused by Tsunami

Poster List

Poster ID	Name	Poster ID	Name
01	Rujun Song	33	Narasak Pandech
02	Surya Velappa Jayaraman_1	34	Gou-Tao Huang
03	Surya Velappa Jayaraman_2	35	Chen-Hao Yeh
04	Syafie Mahmood	36	Thanundon Konknok
05	Darwin Barayang Putungan	37	An Ho
06	Meng-Han Li	38	Duc-Long Nguyen
07	Kun Han Lin	39	Yuwadee Suwan
08	Jeongwoon Hwang	40	Yi En Liu
09	Tun Sriana	41	Icuk Setiyawati
10	Chuan-Hui Zhang	42	Katsumi Hagita
11	Ting Yin Chen	43	W. C. Chen
12	Ting Yi Wei	44	Kai-Hao Tsau
13	Han-Hsin Chiang	45	P. L. Lu
14	Fa-Chieh Chu	46	Yi-Pin Lin
15	Cheng Wei David Gu	47	Chun-Chih Chang
16	Kan Yeep Choo	48	Chen Cheng Liao
17	Jia Cheng Hu	49	Hung Lung Chou
18	Wan-Rou Tong	50	Shiuan-Yau Wu
19	Woosun Jang	51	Chia Ni Li
20	Hong-Guang Xu	52	Jaehyun Bae
21	Hsiao-Han Chuang	53	Amol Deshmukh
22	Jake Acedera Tan	54	Ji-Hwan Lee
23	Liang-Chun Lin	55	Batjargal Sainbileg
24	Kirill V. Gets	56	Alexandra Santos-Putungan
25	Taku Mizukami	57	Muhammad Anshar Makhraja
26	Ianatul Khoiroh	58	Swastibrata Bhattacharyya
27	Vijayan Manickam Achari	59	Kittiphong Amnuyswat
28	I-Shou Huang	60	Yonghyuk Lee
29	Wei Lim Chong	61	Jong Hyun Jung
30	Vertika Gautam	62	Chou-Hsun Yang
31	Chia Jen Hsu	63	Bo-Chao Lin
32	Yin Cheng Chen		

Map of NTUST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NTUST Guest House
公館國小
學人一舍
學人二舍
學人三舍
四段四十一巷六十八弄
後門
第一學生宿舍 Dormitory
第三學生宿舍 Dormitory
第二餐廳
第二學生宿舍 Dormitory
臺灣建築科技中心 Taiwan building technology center
警衛室
電資館EE
游泳池 Natatorium
國際交流中心 international friendship center
第三教學大樓 T3
體育館 Gymnasium
醫務室
學生活動中心 Student Center
學務處 Student Affairs Office
第一餐廳
教職員工餐廳
郵局
水池
管理大樓 MA
第三餐廳
第二教學大樓 T2
工程二館E2
工程一館 E1
排球場
基隆路三段一五五巷
台大醫院公館分院
警衛室
停車場 Parking Lot
籃球場
網球場
第四教學大樓 T4
行政大樓 AD
地下停車場入口 Parking Lot
研揚大樓 AAEON Building
司令台
水池
視聽館 AU
圖書館 Library
國際大樓 IB
ACCMS-8
運動場 Stadium
第一教學大樓 T1
綜合研究大樓 RB
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Keelung Rd.
National Taiwan University