TRACK 2: COMPUTATIONAL CHEMISTRY		
Date 1: July 25th, 2019 ***Venue: Ballroom #1***		
Session 1: Machine learning **Chair: Thanh Tung Nguyen Dang**		
Time	**Agenda**	**Code**
13:30 14:00	**Computational Chemistry and Machine Learning for Nanomedicine** *Nguyen Thi Van Oanh*	CC-01
14:00 14:30	**Predicting new Lanthanide Transition-metal Compound by Machine Learning** *Tien-Lam Pham*	CC-02
14:30 15:00	**Statistical Fragmentation of Molecules** *Dominik Domin*	CC-03
15:00 15:30	Coffee break	
Session 2: Theory – Computer **Chair: Nguyen The Toan**		
Time	**Agenda**	**Code**
15:30 16:00	**Judging density functionals using database: Comments on using statistics** *Andreas Savin*	CC-04
16:00 16:30	**Superconvergent Perturbation Series for the Analytical Resummation of Non-Adiabatic Couplings** *T. Tung Nguyen-Dang*	CC-05
16:30 17:00	**Vibrational Spectroscopy of Carbon Nanostructures** *Henryk A. Witek*	CC-15
17:00 17:30	**TARA: A development of Large-Scale Generalized HPC Service for Scientific Research in Thailand** *Manaschai Kunaseth*	CC-06
Date 2: July 26th, 2019 ***Venue: Meeting Room #1***		
Session 3: Structure – Reactivity **Chair: Huynh Kim Lam**		
Time	**Agenda**	**Code**
9:10 9:40	**An overview of structure and bonding for tetrylones with Group-13-diyls in transition metal complexes** *Nguyen Thi Ai Nhung*	CC-08
9:40 10:10	**Pressure-Dependent Rate Constant Caused by Tunneling Effects: OH + HNO_3 as an Example** *Thanh Lam Nguyen*	CC-09
10:10 10:40	**Quantitative Determination of Photochemistry from First Principles** *Daniel Escudero*	CC-10
10:40 11:00	Coffee break	
11:00 12:00	**Poster session** *Venue: Ballroom #1*	
Session 4: AI - Solution - Solid State **Chair: Pham Ho My Phuong**		
Time	**Agenda**	**Code**
13:30 14:00	**Exploring Physical and Chemical Space of Molecular Systems: Human and/or Artificial Intelligence** *Jer-Lai Kuo*	CC-07

14:00 14:30	**Contribution of Polarizable Force Fields to the Physicochemical Description of the Interaction of Ions with their Environment** *Carine Clavaguéra*	CC-11
14:30 15:00	**Theory of High-Harmonic Generation in Solids: A Perspective from Atomic and Molecular Strong-Field physics** *Anh-Thu Le*	CC-13
15:00 15:20	Coffee break	
Session 5: Materials **Chair: Ong Phuong Khuong**		
Time	**Agenda**	**Code**
15:20 15:50	**Ab initio Crystal Field for Lanthanides** *Liviu Ungur*	CC-14
15:50 16:20	**Siloles As Optoelectronic Materials: Theoretical and Experimental Design** *Nguyen Thi Minh Hue*	CC-18
16:20 16:50	**Density Functional Theory Study on Effect of External Electric Field on Methane Conversion on IrO_2(110) Surface** *Jyh-Chiang Jiang*	CC-17
16:50 17:20	**Electronic and Optical Properties of Monolayer MoS_2 under the Influences of Polyethyleneimine Adsorption and Pressure** *Do Ngoc Son*	CC-16
17:30 18:00	**Poster Award and Closing Ceremony** *Venue: Grand Ballroom*	