Poster Contributions

P1. The p-conjugated P-flowers C16(PH)8 and C16(PF)8 are potential materials for organic n-type semiconductors

Vu Thi Thu Huong, Truong Ba Tai and Minh Tho Nguyen

Department of Chemistry, University of Leuven, B-3001 Leuven, Belgium

vu.thithuhuong@chem.kuleuven.be

P2. Singly and doubly lithium doped silicon clusters: Geometrical and electronic structures and ionization energies

Nguyen Minh Tam,[1,3] Vu Thi Ngan,[1] Jorg de Haeck,[2] Soumen Bhattacharyy[1,2] Hai Thuy Le,[2] Ewald Janssens,[2] Peter Lievens,[2],* and Minh Tho Nguyen[1],*

[1]*Department of Chemistry, Katholieke Universiteit Leuven, B-3001 Leuven, Belgium*

[2]*Laboratory of Solid State Physics and Magnetism, Katholieke Universiteit Leuven, B-3001 Leuven, Belgium*

[3]*Institute for Computational Science and Technology, Ho Chi Minh City, Vietnam*

ngminhtam1983@yahoo.com.vn

P3. Doping effects on the singlet-triplet gap and bonding of the silicon trimer

Nguyen Minh Tam,[1,2] Tran Dieu Hang,[2] Hung Tan Pham,[1] My Phuong Pham-Ho,[1] and Minh Tho Nguyen,[1]

[1]*Institute for Computational Science and Technology (ICST), Quang Trung Software City, Ho Chi Minh City, Vietnam*

[2]*Department of Chemistry, University of Leuven, B-3001 Leuven, Belgium*

dieuhang.tran@chem.kuleuven.be

P4. Effects of Sulfur-Deficient Defect and Water on Rearrangementsof Formamide on Pyrite (100) Surface

Thi Huyen Nguyen, and Minh Tho Nguyen

Department of Chemistry, University of Leuven, B-3001 Leuven, Belgium

thihuyen.nguyen@chem.kuleuven.be

P5. Surface states of the topological crystalline insulator Pb0.4Sn0.6Te

S. Safai, P. Kacman, and R. Buczko

Institute of Physics PAS, al. Lotników 32/46, 02-668 Warsaw, Poland

safai@ifpan.edu.pl

P6. Dual effect of crowders on fibrillation kinetics of polypeptide chains revealed by lattice models

Nguyen Truong Co[1] and Mai Suan Li[2]

[1]*Institute for Computational Science and Technology, SBI Building, Quang Trung Software City, Tan Chanh Hiep Ward, District 12, Ho Chi Minh City, Vietnam*

[2]*Institute of Physics, Polish Academy of Science, Al. Lotnikow 32/46, 02-668 Warsaw, Poland*

truongcophysics@gmail.com

P7. In silico and in vitro characterization of anti-amyloidogenic activity of vitamin K3 analogues for Alzheimer's disease

Pham Dinh Quoc Huy[1,2] and Mai Suan Li[2]

[1]*Institute for Computational Science and Technology, SBI Building, Quang Trung Software City, Tan Chanh Hiep Ward, District 12, Ho Chi Minh City, Vietnam*

[2]*Institute of Physics, Polish Academy of Science, Al. Lotnikow 32/46, 02-668 Warsaw, Poland*

quochuy@ifpan.edu.pl

P8. Analysis of Binding Affinity of Protein-Ligand Complexes

Son Tung Ngo[1,2] and Mai Suan Li[2]

[1]*Institute for Computational Science and Technology, SBI Building, Quang Trung Software City, Tan Chanh Hiep Ward, District 12, Ho Chi Minh City, Vietnam*

[2]*Institute of Physics, Polish Academy of Science, Al. Lotnikow 32/46, 02-668 Warsaw, Poland*

nstung@ifpan.edu.pl

P9. Estimation of the Binding Free Energy of AC1NX476 to HIV-1 Protease Wild-Type and Mutations Using Free Energy Perturbation method

Son Tung Ngo,[1,2] Binh Khanh Mai,[3] Dinh Minh Hiep,[4] and Mai Suan Li[1]

[1]*Institute for Computational Science and Technology, 6 Quarter, Linh Trung Ward, Thu Duc District, Ho Chi Minh City, Vietnam,*

[2]*Institute of Physics, Polish Academy of Sciences, Al. Lotnikow 32/46, 02-668 Warsaw, Poland,*

[3]*Department of Applied Chemistry, College of Applied Sciences, Kyung Hee University, Yongin 446-701, Korea*

[4]*Department of Sciences and Technology, Ho Chi Minh City, Vietnam*

nstung@ifpan.edu.pl

P10. Binding of fullerene to amyloid beta fibrils: Size matters

Pham Dinh Quoc Huy[1,2] and Mai Suan Li[2]

[1]*Institute for Computational Science and Technology, SBI Building, Quang Trung Software City, Tan Chanh Hiep Ward, District 12, Ho Chi Minh City, Vietnam*

[2]*Institute of Physics, Polish Academy of Science, Al. Lotnikow 32/46, 02-668 Warsaw, Poland*

quochuy@ifpan.edu.pl