The 4th China-Japan-Korea Workshop on Theoretical and Computational Chemistry (CJK-WTCC-IV)

CONFERENCE PROGRAM

Nanjing • China

January 9-13, 2019

ACKNOWLEDGEMENTS

The organizing committee expresses its gratitude to Nanjing University for hosting this conference. Special thanks are given to "Jiangsu Society of Chemistry and Chemical Engineering (JSSCCE)" for co-organizing this conference. We thank all of the volunteers who contribute to the success of this meeting.

Conference URL: http://itcc.nju.edu.cn/cjkwtcc4

The 4th China-Japan-Korea Workshop on Theoretical and Computational Chemistry

THE STEERING COMMITTEE:

Wenjian Liu, Peking University, China

Weihai Fang, Beijing Normal University, China

Shuhua Li, Nanjing University, China

Hiromi Nakai, Waseda University, Japan

Takahito Nakajima, RIKEN Advanced Institute for Computational Science, Japan

Shinji Saito, Institute for Molecular Science, Japan

Jin Yong Lee, Sungkyunkwan University, Korea

Cheol Ho Choi, Kyungpook National University, Korea

Young Min Rhee, POSTECH, Korea

THE LOCAL ORGANIZING COMMITTEE:

Shuhua Li (chairman)

Daiqian Xie

Zhaoxu Chen

Haibo Ma

Yanzi Zhou

Chunfeng Zhang

Weihai Fang

Jing Ma

Chungen Liu

Wei Li

Hao Dong

Conference Site

Nanjing University International Conference Center (**NUICC**) is located in Nanjing University Xianlin Campus, close to the east gate. The distance from the airport/railway station/metro station to the NUICC is

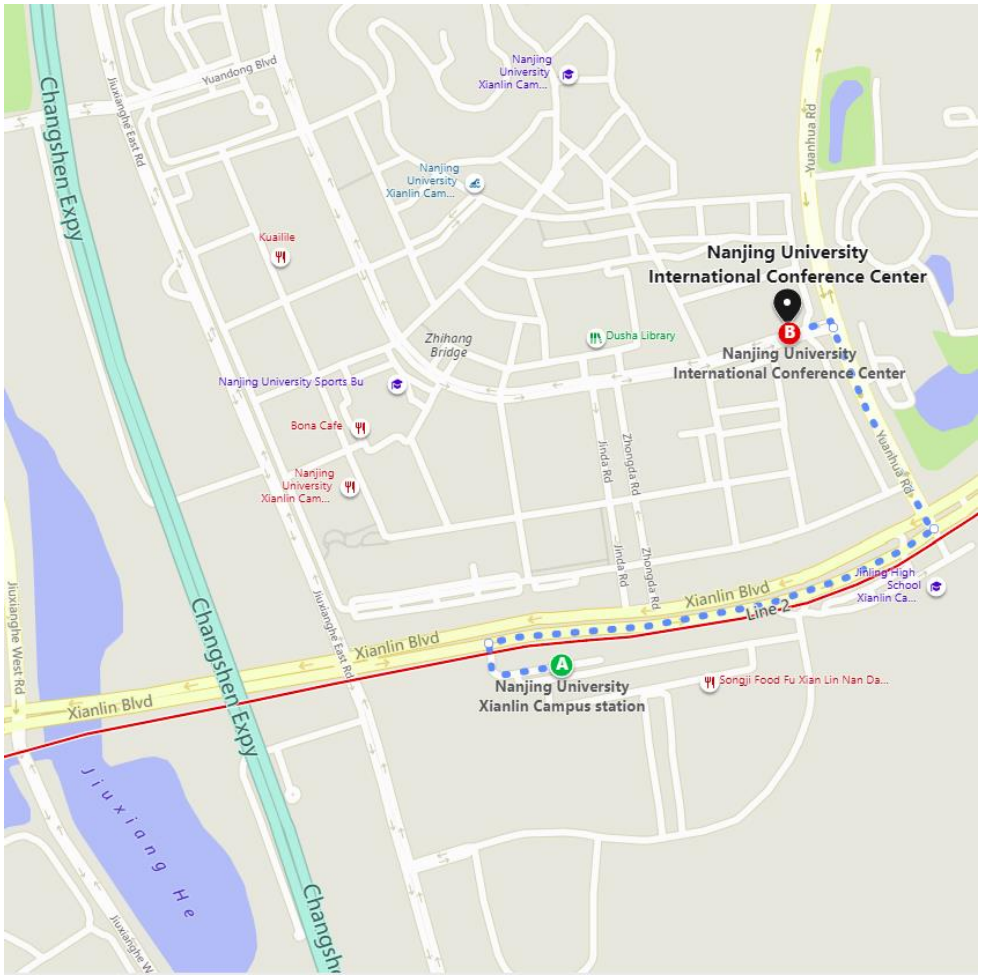
Location	distance/km
Nanjing Railway Station	21
Nanjing South Railway Station	32
Nanjing Lukou International Airport	65

(Note: The "Nanjing Railway Station" is different from the "Nanjing South Railway Station", and the distance between two stations is about 30 min's drive)

Please show the following card to the taxi driver in case he or she cannot speak English.

请送我去南京大学国际会议中心(栖霞区仙林大道163号)

Please take me to the Nanjing University International Conference Center (163 Xianlin Avenue, Qixia District)



A: Nanjing University Xianlin Campus Station (Metro Line 2)
B: Nanjing University International Conference Center (NUICC)

Information

Registration, welcome reception, talk sessions, poster session, lunches, and dinners will be in the Nanjing University International Conference Center (NUICC).

Registration: 1st floor of NUICC

Welcome reception: Room 301 in the 3rd floor of NUICC

Talk sessions: Zhongda Hall in the 2nd floor of NUICC

Poster session: outside of Zhongda Hall in the 2nd floor of NUICC

Lunches & dinners: 1st floor of NUICC

Banquet (for invited guests): Houmen Hall at Mandarin Garden Hotel in the area of Confucius Temple

Contacts

Name	Mobile	Email	Note
Shuhua Li	135-8402-9625	shuhua@nju.edu.cn	Chair
Wei Li	182-0514-7575	wli@nju.edu.cn	Registration/Accommodation
Haibo Ma	189-1478-8480	haibo@nju.edu.cn	Conference Facilities
Hao Dong	139-1395-2818	donghao@nju.edu.cn	Transportation
Chunfeng Zhang	133-3780-6766	cfzhang@nju.edu.cn	Excursion

General Program

	Jan 9 (Wed)	Jan 10 (Thu)	Jan 11 (Fri)	Jan 12 (Sat)
08:50-09:00		Opening Remark		
		Chair: Jinlong Yang	Chair: Weihai Fang	Chair: Jian Liu
09:00-09:50		Yuki Kurashige	Jong-Won Song	Masahiro Higashi
09:50-10:40		Jae Woo Park	Igor Ying Zhang	Chang Woo Kim
10:40-11:00		Group photo & Tea Break	Tea Break	Tea Break
		Chair: Hiromi Nakai	Chair: Linjun Wang	Chair: Ganglong Cui
11:00-11:50		Bingbing Suo	Ryohei Kishi	Qian Peng
11:50-14:00		Lunch	Lunch	Lunch
		Chair: Jin Yong Lee		Chair: Zhenggang Lan
14:00-14:50	Arrival&	Zhenyu Li	Free time	Geunsik Lee
14:50-15:40	Check-in	Sunkyung Kim		Peifeng Su
15:40-16:00		Tea Break		Tea Break
		Chair: Haibo Ma		Chair: Wenjian Liu
16:00-16:50		Naoki Nakatani		Chien-Pin Chou
16:50-17:40		Lin Shen		Panel Discussion
17:50-19:00	Welcome	Dinner	Banquet (18:30-)	Dinner
19:00-20:00	reception	Poster Session	(invited guests)	
20:00-21:00				

Scientific Program

Jan 10 (Thu)	Zhongda Hall, NUICC (2nd floor)
08:50-09:00	**Opening Remark**
Session I	**Chair: Jinlong Yang (University of Science and Technology of China)**
09:00-09:50	Yuki Kurashige (Kyoto University)
	Excited-state quantum dynamics with time-dependent matrix-product states
09:50-10:40	Jae Woo Park (Chungbuk National University)
	CASPT2 photochemistry: gradient, derivative coupling, and conical intersections
10:40-11:00	Group photo & Tea Break
Session II	**Chair: Hiromi Nakai (Waseda University)**
11:00-11:50	Bingbing Suo (Northwest University)
	New development of Beijing Density Functional package and its applications
11:50-14:00	Lunch (1st floor of NUICC)
Session III	**Chair: Jin Yong Lee (Sungkyunkwan University)**
14:00-14:50	Zhenyu Li (University of Science and Technology of China)
	Atomistic simulation of reaction and growth on surface
14:50-15:40	Sunkyung Kim (Air Force Academy of Korea)
	Catalytic activity of TiO2 nanoparticles with oxygen vacancy
15:40-16:00	Tea Break
Session IV	**Chair: Haibo Ma (Nanjing University)**
16:00-16:50	Naoki Nakatani (Tokyo Metropolitan University)
	Theoretical studies on the XANES spectra of transition metal complexes
16:50-17:40	Lin Shen (Beijing Normal University)
	Development of quantum mechanics/molecular mechanics method combined with resolution-adapted and neural network models
17:50-19:00	Dinner
19:00-21:00	**Poster Session** (Outside of Zhongda Hall, NUICC, 2nd floor)

Jan 11 (Fri)	Zhongda Hall, NUICC (2nd floor)
Session V	**Chair: Weihai Fang (Beijing Normal University)**
09:00-09:50	Jong-Won Song (Daegu University)
	Development of DFT functional applicable to large molecular and periodic systems
09:50-10:40	Igor Ying Zhang (Fudan University)
	Towards efficient orbital-dependent density functional approximation for molecular and periodic systems
10:40-11:00	Tea Break
Session VI	**Chair: Linjun Wang (Zhejiang University)**
11:00-11:50	Ryohei Kishi (Osaka University)
	Molecular and periodic systems with open-shell electronic structures: From geometric and energetic features to response properties
11:50-14:00	Lunch (1st floor of NUICC)

Jan 12 (Sat)	Zhongda Hall, NUICC (2nd floor)
Session VII	**Chair: Jian Liu (Peking University)**
09:00-09:50	Masahiro Higashi (University of the Ryukyus)
	Toward a molecular understanding of excitation energy transfer in light-harvesting complexes
09:50-10:40	Chang Woo Kim (Korea Advanced Institute of Science and Technology, KAIST)
	Toward quantum chemical description of photodynamics in light-harvesting complexes with interpolated molecular potential
10:40-11:00	Tea Break
Session VIII	**Chair: Ganglong Cui (Beijing Normal University)**
11:00-11:50	Qian Peng (Institute of Chemistry, Chinese Academy of Sciences)
	Excited state process in organic light-emitting materials
11:50-14:00	Lunch (1st floor of NUICC)
Session IX	**Chair: Zhenggang Lan (South China Normal University)**
14:00-14:50	Geunsik Lee (Ulsan National Institute of Science and Technology, UNIST)
	Effects of organic cation and electrode junction on electronic structures of $MAPbI_3$
14:50-15:40	Peifeng Su (Xiamen University)
	Generalized Kohn-Sham energy decomposition analysis scheme (GKS-EDA) and its applications
15:40-16:00	Tea Break
Session X	**Chair: Wenjian Liu (Peking University)**
16:00-16:50	Chien-Pin Chou (Waseda University)
	Development of automatized density-functional tight-binding parameterization
16:50-17:30	Panel Discussion
17:50-19:00	Dinner

Poster Program

Jan 10	19:00-21:00: Outside of Zhongda Hall, NUICC (2nd floor)
P-01	**Linjun Wang** (Zhejiang University)
	Methods for Crossing and Decoherence Corrections
P-02	**Ye Mei** (East China Normal University)
	Acceleration of QM/MM free energy calculations
P-03	**Yanan Guo** (Nanjing Tech University)
	Different hydrogen bonding environments of the retinal protonated Schiff base control the photoisomerization in Channelrhodopsin-2
P-04	**Zhaoxu Chen** (Nanjing University)
	ReaxFF Molecular Dynamics Simulations of Pd/ZnO Systems
P-05	**Haibo Ma** (Nanjing University)
	Nonadiabatic Exciton Dynamics by Time-Dependent Density Matrix Renormalization Group
P-06	**Hao Dong** (Nanjing University)
	Principles Governing Catalytic Activity of Self-Assembled Short Peptides
P-07	**Wei Li** (Nanjing University)
	Generalized Energy-Based Fragmentation Approach for Energies and Spectroscopy of Large Systems
P-08	**Yuanjun Gao** (Beijing Normal University)
	Theoretical Studies on the Mechanism of Thermally Activated Delayed Fluorescence in Organometallic Complexes
P-09	**Pin Xiao** (Beijing Normal University)
	Mechanism of Light-Driven Aerobic Oxidative Coupling of Phenols and Alkynes by Copper Photocatalyst
P-10	**Feng An** (Nanjing University)
	Quantum Dynamics of the Quenching Reaction CNN
P-11	**Fangjia Fu** (Nanjing University)
	How intermolecular interactions influence electronic absorption spectra: insights from the molecular packing of uracil in condensed phases
P-12	**Théophile Gaudin** (Nanjing University)
	Predicting dielectric constant of organic liquids based on molecular surfaces
P-13	**Jing Huang** (Nanjing University)
	Theoretical calculations of potential energy surfaces for several vdW complexes containing HF molecule
P-14	**Zhen Luo** (Nanjing University)
	Externally-Contracted Multi-Reference Configuration Interaction Method Using a DMRG Reference Wave Function
P-15	**Zhigang Ni** (Nanjing University)
	Further Development in the Cluster-in-Molecule Local Correlation Approach for Large Systems
P-16	**Harikrishna Sahu** (Nanjing University)
	Designing Promising Molecules for Organic Solar Cells via Machine Learning Assisted Virtual Screening

P-17	**Qingchun Wang** (Nanjing University)
	Automatic Construction of the Initial Orbitals for Efficient Generalized Valence Bond Calculations of Large Systems
P-18	**Xiaoyu Xie** (Nanjing University)
	An exciton-phonon interaction model for singlet fission in prototypical molecular crystals
P-19	**Daibei Yang** (Nanjing University)
	Rational Design of One-Dimensional Hybrid Organic-Inorganic Perovskites with Excellent Ferroelectricity and Piezoelectricity
P-20	**Manyi Yang** (Nanjing University)
	Combined Molecular Dynamics and Coordinate Driving Method for Automatic Reaction Pathway Search of Reactions in the Solution
P-21	**Dandan Yuan** (Nanjing University)
	Structures and properties of large supramolecular coordination complexes predicted with the generalized energy-based fragmentation method
P-22	**Dongbo Zhao** (Nanjing University)
	Accurate Prediction of NMR Chemical Shifts in Macromolecular and Condensed-Phase Systems with the Generalized Energy-Based Fragmentation Method
P-23	**Qiang Zhu** (Nanjing University)
	Partition of Drug-like Molecules in Biological Membrane
P-24	**Qiang Zhu** (Nanjing University)
	A Data-Driven Accelerated Sampling Method for searching Functional States of Proteins

Notes for Posters

Excited-State Quantum Dynamics with Time-Dependent Matrix-Product States

Yuki Kurashige*

Department of Chemistry, Graduate School of Science, Kyoto University
Kitashirakawa Oiwake-cho, Sakyo-ku Kyoto, 606-8502, Japan
*Email: kura@kuchem.kyoto-u.ac.jp

A matrix product state formulation of the multiconfiguration time-dependent Hartree (MPS-MCTDH) theory will be presented. The Hilbert space that is spanned by the direct products of the phonon degree of freedoms, which is linearly parameterized in the MCTDH ansatz and thus results in an exponential increase of the computational cost, is parametrized by the MPS form. Equations of motion based on the Dirac-Frenkel time-dependent variational principle is derived by using the tangent space projection and the projector-splitting technique for the MPS, which have been recently developed. The mean-field operators, which appear in the equation of motion of the MCTDH single particle functions (SPF), are written in terms of the MPS form and efficiently evaluated by a sweep algorithm that is similar to the DMRG sweep. The efficiency and convergence of the MPS approximation to the MCTDH are demonstrated by quantum dynamics simulations of extended excitonic molecular systems.

[1] Yuki Kurashige, "Matrix product state formulation of the multiconfiguration time-dependent Hartree theory" *J Chem Phys* in press (2018).
[2] Yuki Kurashige, "Multireference electron correlation methods with density matrix renormalisation group reference functions" *Mol Phys* **112,** 1485–1494 (2014).
[3] Yuki Kurashige and Takeshi Yanai, "Second-order perturbation theory with a density matrix renormalization group self-consistent field reference function: Theory and application to the study of chromium dimer" *J Chem Phys* **135,** 094104 (2011).
[4] Yuki Kurashige and Takeshi Yanai, "High-performance *ab initio* density matrix renormalization group method: applicability to large-scale multireference problems for metal compounds" *J Chem Phys* **130,** 234114 (2009).

Notes

CASPT2 photochemistry: gradient, derivative coupling, and conical intersections

Jae Woo Park*

Department of Chemistry, Chungbuk National University, Cheongju, Korea
*Email: jaewoopark@cbnu.ac.kr

Second-order complete active space perturbation theory (CASPT2) is one of the most efficient ab initio methods toward accurate descriptions of both static and dynamical electronic correlations. Here, I will talk about recent progress in CASPT2 to calculate excited states potential energy surfaces and the surface crossings between excited states and the ground state. In particular, the automatic code generation technique has been used to simplify and implement tensor operations in the CASPT2 formalism. With these developments, locating conical intersections of molecules with >50 atoms and performing molecular dynamics simulations with >20 atoms are now routine. I will also discuss some practical issues of the CASPT2 calculations for calculating excited states, such as selections of zeroth-order Hamiltonian and level shifts.

Notes

New Development of Beijing Density Functional Package and Its Applications

Bingbing Suo,[a,*] Yibo Lei,[a] Yong Zhang,[b] Wenjian Liu[b]

a) Institute of Modern Physics, Northwest University, Xi'an, Shanxi 710127, China
b) College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China

Beijing Density Functional package (BDF) is a general-purpose quantum chemistry package developed in Chinese Quantum Chemistry Society.[1] In this lecture, I will introduce some recent progresses in developing of BDF package. Firstly, Some special theories and algorithms first implemented in BDF package will be presented. Then, linear scaling DFT/TDDFT in BDF will be presented. By combining the multi-pole expansion to treat the Coulomb interaction and semi-numerical integral algorithm to calculate the Hartree-Fock exchange, computational times of DFT/TDDFT are reduced significantly while the accuracy could be guaranteed. BDF has used to study the emission mechanism of the open-shell radical molecule in organic light emission device (OLED).[2] The puzzle of 100% internal quantum efficiency (IQE) in the radical emitter is revealed. Finally, internally contracted multi-reference configuration interaction with single and double excitation (icMRCISD) and multi-state n-electron valance second order perturbation theory (MS-NVEPT2) based on graphical unitary group approach (GUGA) will be presented. [3] Both icMRCISD and MR-NEVPT2 are implemented in Xi'an-CI package and have been interfaced with BDF.[1,3]

[1] BDFwiki, http://182.92.69.169:7227
[2] C. He, Z. Li, W. Zou, Y. Lei, B. Suo, Manuscript submitted.
[3] B. Suo, Y. Lei, H. Han, Y, Wang, Mole. Phys., **116**, 1051-1065,2018.

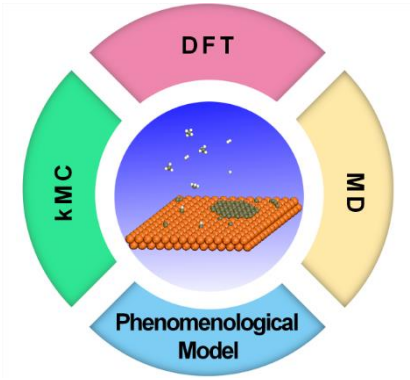
Notes

Atomistic Simulation of Reaction and Growth on Surface

Zhenyu Li

Hefei National Laboratory for Physical Sciences at Microscale, University of Science and Technology of China, Hefei, 230026, China
Email: zyli@ustc.edu.cn

Atomistic details are usually difficult to obtain *in situ* during complicated surface processes. Therefore, direct atomistic simulations, although very challenging, are highly desirable.[1] Typically, efficient algorithms should be developed to speed up the simulation and clever models should be designed to dig out the physical picture behind simulation data.



Graphene is an important material with unique properties and accordingly many potential applications. A promising way to produce high-quality wafer-size graphene is chemical vapor deposition (CVD) on metal surfaces. To improve the sample quality, it is important to understand the atomic mechanisms of graphene growth. Why byproduct H_2 should be provided in CVD growth of graphene has been answered by kMC simulations at experimental conditions.

Kinetic parameters of the elementary reactions should be provided in kMC simulations, which are typically obtained from minimum energy path search. However, at very high temperature, it is not known if such a protocol can give reliable kinetic parameters. For this purpose, methane decomposition on Cu(111) has been studied by ab initio molecular dynamics (AIMD). Useful insights about high temperature surface reaction have been obtained.

[1] Zongyang Qiu, Pai Li, Zhenyu Li,* and Jinlong Yang, *Atomistic Simulations of Graphene Growth: From Kinetics to Mechanism*, Acc. Chem. Res., **51**, 728 (2017).

Notes

Catalytic activity of TiO_2 nanoparticles with oxygen vacancy

Sunkyung Kim[a)], Kyoung Chul Ko[b)], Jin Yong Lee[c)*] and Francesc Illas[d)*]

a) Department of Basic Science, Korea Air Force Academy, Cheongju 28187, Korea
b) Department of Chemistry Education, Chonnam National University, Gwang-ju 61186, Korea
c) Department of Chemistry, Sungkyunkwan University, Suwon 16419, Korea
d) Departament de Quı´mica Fı´sica & Institut de Quı´mica Teo`rica i Computacional (IQTCUB), Universitat de Barcelona, 08028 Barcelona, Spain

[*]Email: jinylee@skku.edu, francesc.illas@ub.edu

Titanium dioxide (TiO_2), as a semiconductor metal oxide, has been one of the most popular materials studied in the field of photocatalysis. The properties of oxygen vacancy in $(TiO_2)_{35}$ nanoparticle were investigated by DFT calculations. $(TiO_2)_{35}$ is the minimum sized model for a bipyramidal nanoparticle with anatase phase and eight {101} facets. The structure of pristine $(TiO_2)_{35}$ is somewhat different from the bulk lattice, with a relatively high surface to volume ratio. The geometric, energetic and electronic properties of the reduced TiO_2 clusters were analyzed by hybrid DFT functionals with different Hartree–Fock exchange ratios (0, 12.5 and 25%). The properties of oxygen vacancy in the $(TiO_2)_{35}$ nanoparticle depend on % Fock of the functional used. The number of vacancy (one or two) and the position of vacant sites were also considered. The vacancy formation energies and the band edge energy levels of the defect state are quite dependent on vacant sites. When the O atom is removed from some specific sites, the oxygen vacancy formation energy is surprisingly small compared with that of the bulk or slab surface. This is because of the relaxation of the reduced TiO_2 system upon vacancy formation. The defect states of reduced nanoparticle are appeared at 0.47 ~ 2.06 eV range below unoccupied molecular orbital (LUMO) energy level and it increases with the number of removed O atoms. And the energies of the defect states induced by an O vacancy are close to the oxygen evolution potential. These results could provide evidence of the importance of the oxygen vacancy of TiO_2 nanoparticles for efficient photocatalysis.

[1] S. Kim, K. C. Ko, J. Y. Lee, and F. Illas, Phys. Chem. Chem. Phys., **18**(34), 23755 (2016).

Notes

Theoretical studies on the XANES spectra of transition metal complexes

Naoki Nakatani,* Jun Yi, and Masahiko Hada

Department of Chemistry, Graduate School of Science, Tokyo Metropolitan University, Tokyo, 192-0397, Japan

*Email: naokin@tmu.ac.jp

X-ray absorption spectroscopy (XAS) is known as a useful tool to experimentally observe local structure and electronic state of a wide variety of molecules with atomic resolution. In particular, it is applicable to non-crystalline materials for which X-ray diffraction (XRD) is not available, and/or paramagnetic molecules for which nuclear magnetic resonance (NMR) spectroscopy is problematic.

However, because the spectrum analysis of XAS is often very complicated, it requires professional knowledge and experience of XAS and/or depends on many parameters to fit the experimental spectra. Thus, a parameter-free analysis based on quantum chemistry calculation is to be very powerful tool to obtain a highly accurate structural and electronic state information from the XAS spectra.

In this work, we theoretically investigated the vanadium *K*-edge and iron $L_{2,3}$-edge spectra of molecular catalyses, to reveal the structures and electronic states of intermediates in solution phase. We employed the TD-DFT and RASSCF/RASPT2 methods to compute the pre-edge region of XAS spectra, known as XANES (X-ray absorption near-edge structure), which involves a lot of information about valence electrons.

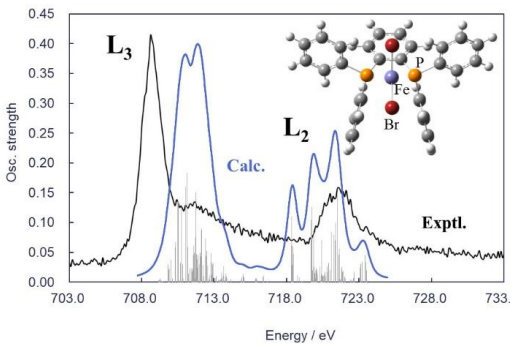


Figure 1. Calculated core-excitation spectra of $FeBr_2SciOPP$ (blue) and XANES spectra from the experiment (black)

Figure 1 shows the experimental and calculated L_3 and L_2 spectra of [$FeBr_2SciOPP$] which is a stable precursor of cross-coupling catalyst reported by Takaya and co-workers. It is clear that the calculated spectra (blue) qualitatively reproduced the experimental spectra (black) without any empirical parameters.

Experimental data only shows two large peaks with small shoulder peaks. However, the calculated spectra indicate that they consist of a lot of peaks reflecting a complicated electronic structure arises from the iron centre. The first-peak (L_3) is about 3 eV overestimated in the calculated spectra. This is originated from insufficient basis functions for a core-hole state and missing electron correlation. The second-peak (L_2) appears mainly due to the spin-orbit coupling of the 2p orbitals. The calculated spectra qualitatively agree with the experimental one although the splitting width was slightly underestimated.

Consequently, our approach to simulate the XAS spectra would be quite useful to analyse the experimental spectra and to obtain detailed information about the geometry and electronic structure coupled with experimental observation.

Notes

Development of QM/MM Method combined with Resolution-Adapted and Neural Network Models

Lin Shen [a)], Hao Hu [b)], and Weitao Yang [c)]

a) Key Laboratory of Theoretical and Computational Photochemistry, Ministry of Education, College of Chemistry, Beijing Normal University, Beijing 100875, P.R.China
b) Department of Chemistry, The University of Hong Kong, Hong Kong, P.R.China
c) Department of Chemistry, Duke University, Durham, NC 27708, United States

[*]Email: lshen@bnu.edu.cn

Because of the significant change in electronic structures of complex systems with a large number of degrees of freedom, the combined quantum mechanical and molecular mechanical (QM/MM) method is an accurate and computationally efficient tool toward QM descriptions on realistic chemical and biological reactions. Based on the potential energy calculations, direct molecular dynamics (MD) simulation using QM/MM model is very powerful for studying the mechanism of reactions in a complex environment but also very time-consuming. The research in the field of QM/MM MD by now still faces many challenges, such as the slow sampling for the MM subsystem and the demanding cost on the QM subsystem. To address the first issue, we developed a resolution-adapted method that spans three levels of resolution as quantum mechanical, all-atomic (AA) and coarse-grained (CG) models [1,2]. The resolution-adapted AA+CG force field for water, in which the interactions between two water molecules are adjusted automatically according to their distance while an all-atom structural description of the entire system is maintained during MD sampling, is applied to QM/MM approach to calculate redox potentials of aqueous metal complexes. The improvements on accuracy and efficiency highlight the importance of a sophisticated MM model. To address the second issue, we developed a neural network (NN) method for ab initio QM/MM MD simulations [3,4]. Using machine learning techniques, the QM/MM potential energy of any configuration for a given reaction system in a complex environment is predicted at the ab initio level based on semiempirical QM/MM MD sampling, and the saving in computational cost is about two orders of magnitude. Combined with an adaptive procedure for NN models, direct MD simulation on the NN-predicted potential energy surface is implemented to approximate ab initio QM/MM MD. The free energy profiles can be reproduced at the ab initio QM/MM accuracy yet at the computational cost as small as the semiempirical QM/MM models. We also discuss the possibility to extend our new methods to excited state QM/MM calculation and nonadiabatic MD simulation in order to study a broad range of problems in photochemistry.

[1] L. Shen and H. Hu, *J. Chem. Theory Comput.*, **10**, 2528 (2014).
[2] L. Shen and W. Yang, *J. Chem. Theory Comput.*, **12**, 2017 (2016).
[3] L. Shen, J. Wu, and W. Yang, *J. Chem. Theory Comput.*, **12**, 4934 (2016).
[4] L. Shen and W. Yang, *J. Chem. Theory Comput.*, **14**, 1442 (2018).

Notes

Development of DFT functional applicable to large molecular and periodic systems

Jong-Won Song[a,*]

a) Chemistry Education, Daegu University, 201 Daegudae-ro, 38453 Republic of Korea
[*]Email: sjoshua@daegu.ac.kr

Nowadays, density functional theory (DFT) is a strong work-horse applicable to biomolecule and material sciences. In particular, hybrid DFT functionals which include Hartree-Fock (HF) exchange in exchange functional initiated active chemical applications of DFT, in that it can reproduce energy and property of finite systems within chemical accuracy as well as with low computational. However, in spite of its high applicability, DFT has shown severe inappropriateness of producing some following basic properties: inter- and intra-molecular van der Waals interaction, inter- and intra-molecular charge transfer excitation energy and its oscillator strength, (hyper-)polarizability, isomerization energy of organic molecules, core-excitation energy, HOMO-LUMO gaps of molecules, and so on. As a result of our commission to solve these problems, we proposed a new hybrid functional named long-range corrected (LC) DFT and showed successful improvement on the problems mentioned above [1].

However, still high demanding of time cost to evaluate long-range HF exchange is a obstacle for LC-DFT to be applied to large molecular systems and solid-state materials. Unlike acceleration methods for Coulomb integration, developing acceleration methods for the HF exchange is still a pioneering area. Upon this problem, we sudied on developing a new linear-scaling method of HF exchange integration, in particular, for LC-DFT hybrid functional [2]. Then, we successfully applied our accelerated LC-DFT to the adsorption energy calculations of CO molecule on Cu periodic surface [3] and found LC-DFT functionals can reproduce the experimental adsorption energies with high selectivity on binding site, not to mention surface energies and lattice energies.

In addition to these topics, recent studies on isomerization energy calculations using LC-DFT with week interaction correlation and carbon nano tube binding site calculations will also be presented.

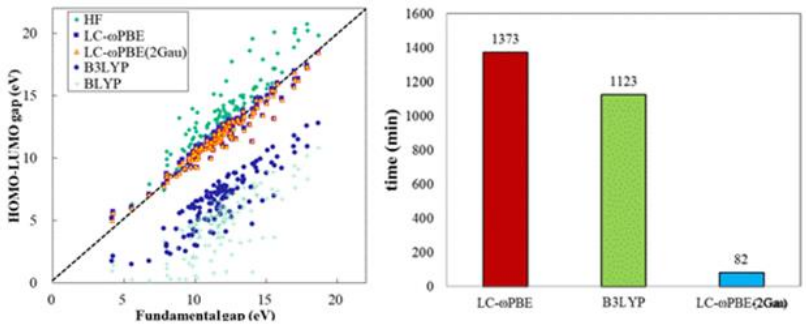


Figure 1: (left) Reference fundamental gap vs HOMO-LUMO gap calculated (right) timings for 1 cycle periodic diamond using various DFT methods and LC-DFT(2Gau)

[1] J.-W. Song, T. Hirosawa, T. Tsuneda, and K. Hirao, J. Chem. Phys. **126**, 154105 (2007).

[2] J.-W. Song and K. Hirao, J. Chem. Phys. **143**, 144112 (2015).

[3] J.-W. Song and K. Hirao, to be submitted.

Notes

Towards efficient orbital-dependent density functional approximation for molecular and periodic systems

Igor Ying Zhang[a,*]

[a]Department of Chemistry, Fudan University, Shanghai, 200438, P.R.China
*Email:igor_zhangying@fudan.edu.cn

Despite a great success of semi-local density functional approximations (DFA) in physics, chemistry, and materials science, these functionals have reached a limit of accuracy where any improvement over several well-documented failures cannot be achieved without a worsening elsewhere. These failures include unsatisfactory predictions of atomization energies, significant underestimations of weak interactions and reaction barriers, and thein capability in describing molecular dissociations and other systems with remarkable multi-reference nature. In this presentation, I will show some of my works in the construction of advanced DFAs which employ the unoccupied as well as the occupied Kohn-Sham orbitals. These functionals were constructed and rationalized in the adiabatic-connection framework,[1–4] exhibiting a significant improvement over conventional DFAs for the aforementioned failures. Relevant developments were made focusing on the computational efficiency of these advanced DFAs and the applicability of these methods in periodic boundary conditions.[5]

[1] Y. Zhang, X. Xu, and W. A. Goddard, Proc. Natl. Acad. Sci. USA **106**, 4963 (2009).
[2] I. Y. Zhang, X. Xu, Y. Jung, and W. A. G. Iii, Proc. Natl. Acad. Sci. USA **108**, 19896 (2011).
[3] I. Y. Zhang and X. Xu, J. Phys. Chem. Lett. **4**, 1669 (2013).
[4] I. Y. Zhang, P. Rinke, J. P. Perdew, and M. Scheffler, Phys. Rev. Lett. **117**, 133002 (2016).
[5] I. Y. Zhang, A. J. Logsdail, X. Ren, S. V. Levchenko, L. Ghiringhelli, and M. Scheffler, arXiv:1808.09780 [cond-mat, physics:physics] (2018), 1808.09780.

Notes

Molecular and Periodic Systems with Open-Shell Electronic Structures: From Geometric and Energetic Features to Response Properties

Ryohei Kishi*[a)]

a) Graduate School of Engineering Science, Osaka University, 1-3 Machikaneyama, Toyonaka, Osaka 560-8531, Japan
*Email: rkishi@cheng.es.osaka-u.ac.jp

Electronic structures of open-shell systems, such as high spin species, excited species, reaction intermediates, polycyclic hydrocarbons, transition metal complexes, etc., are expected to be sensitive to the external physical and chemical perturbations, the feature of which can be reflected in their high reactivity and unique magnetic and optical response properties. In this regard, molecular designs based on the open-shell electronic structures have attracted intense attentions from the viewpoint of creating novel multi-functional molecular materials. For example, we have theoretically established design guidelines for molecules exhibiting highly efficient third-order nonlinear optical (NLO) properties from the viewpoint of diradical character (y).[1] The value of y, which is defined from the weight of the double excitation in the ground state wavefunction,[2] is related to the instability of an effective chemical bonding. Several practical design strategies for tuning y have also been proposed from the viewpoints of modifying atomic/molecular species (organic, heavy main group and transition metal elements), geometric features (size, shape, planarity, etc.), and chemical structures (σ/π/δ-bondings, aromaticity, delocalization, etc.). From the theoretical approaches, both qualitative and (semi)quantitative descriptions of such electronic structures of a variety of open-shell molecular systems are important. Even though recent progress in the basic theories and computational techniques that can treat open-shell electronic structures is remarkable, their practical applications to geometries, energetics and response properties have not been sufficiently discussed. In this presentation, we will introduce several molecular and periodic systems with open-shell electronic structures, e.g., oligomers with quinoidal structures (Fig. 1a),[3] polycyclic hydrocarbons involving five membered rings,[4] and one-dimensional molecular crystals composed of open-shell singlet molecules (Fig. 1b). On the basis of the theoretical and experimental results, we will discuss applicability of several quantum chemical calculations to the detailed analysis of open-shell electronic structures of such complex molecular systems.

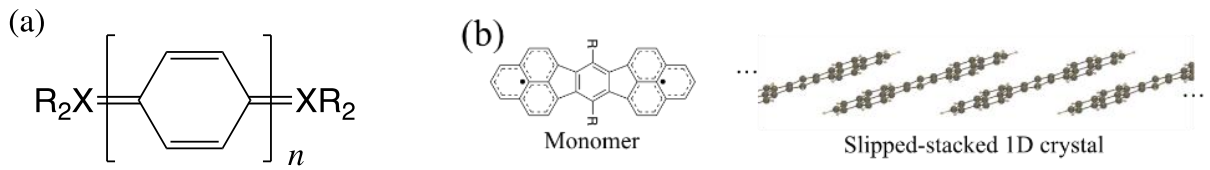


Figure 1: Examples of open-shell molecular systems.

[1] M. Nakano, R. Kishi, et al., Phys. Rev. Lett., **99**, 033001 (2007).

[2] E. F. Hayes, A. K. Q. Siu, J. Am. Chem. Soc., **93**, 2090 (1971); K. Yamaguchi, T. Fueno, H. Fukutome, Chem. Phys. Lett., **22**, 461 (1973).

[3] D. Rottschäfer, J. Busch, B. Neumann, H.-G. Stammler, M. van Gastel, R. Kishi, M. Nakano, R. S. Ghadwal, Chem.-Eur. J. **24**, 16537 (2018).

[4] A. Shimizu, R. Kishi, M. Nakano, D. Shiomi, K. Sato, T. Takui, I. Hisaki, M. Miyata, Y. Tobe, Angew. Chem. Int. Ed., **52**, 6076 (2013).

Notes

Toward a molecular understanding of excitation energy transfer in light-harvesting complexes

Masahiro Higashi[a,b,*]

a) Department of Chemistry, Biology and Marine Science, University of the Ryukyus, 1 Senbaru, Nishihara, Okinawa 903-0213, Japan
b) JST, PRESTO, 4-1-8 Honcho, Kawaguchi, Saitama, 332-0012, Japan
[*]Email: higashi@sci.u-ryukyu.ac.jp

Light-harvesting complexes efficiently transfer absorbed light energy to the reaction center of photosystems. To maximize the efficiency of the energy transfer, the protein environment tunes the excitation energies of pigments, defined as the site energies, and their fluctuations, although the detailed mechanism is unknown. The Fenna− Matthews−Olson (FMO) complex is the first light-harvesting complex to be solved by X-ray crystallography and has extensively been studied experimentally and theoretically. However, none of previous theoretical studies using molecular dynamics (MD) simulations combined with electronic structure calculations cannot reproduce the experimental site energies and their fluctuations quantitatively.

To solve the difficulty, we first have improved the description of excited-state electronic structures of pigment by optimizing the parameter of the CAM-B3LYP density functionals [1]. Next, we have developed the molecular mechanics with Shepard interpolation correction (MMSIC) method to generate an accurate semi-global potential energy surface with low computational cost [2]. By solving these two problems, we can successfully reproduce the site energies and their fluctuations quantitatively (Figure 1). It is found that the excitation energy fluctuations at different sites are significantly different. Population dynamics simulation with hierarchical equations of motion (HEOM) revealed that the site-dependent fluctuations can accelerate the excitation energy transfer rate (Figure 2) [3].

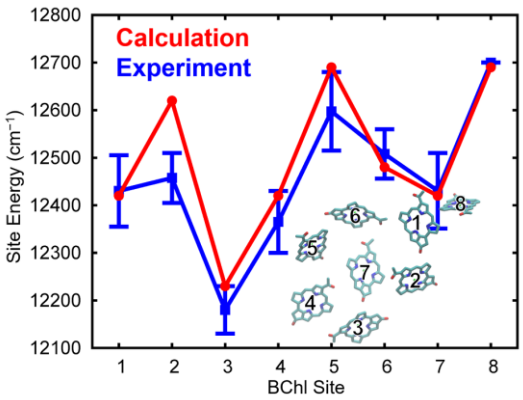


Figure 1. Comparison of the calculated site energies with the experimental ones.

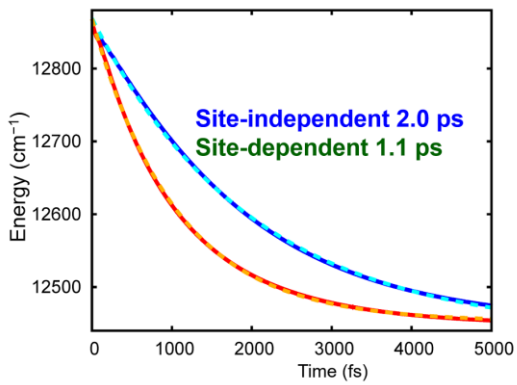


Figure 2. Energy relaxation analysis of population dynamics with the site-

[1] M. Higashi, T. Kosugi, S. Hayashi, and S. Saito, J. Phys. Chem. B, **118**, 10906 (2014).
[2] M. Higashi and S. Saito, J. Chem. Theory Comput., **12**, 4128 (2016).
[3] M. Higashi and S. Saito, in preparation.

Notes

Toward quantum chemical description of photodynamics in light-harvesting complexes with interpolated molecular potential

Chang Woo Kim[a] and Young Min Rhee[a*]

a) Department of Chemistry, Korea Advanced Institute of Science and Technology (KAIST), Daejeon, 34141, Republic of Korea
[*]Email: ymrhee@kaist.ac.kr

Nonadiabatic dynamics in complex molecular systems has been thoroughly studied in recent years due to its potential importance in biological and material sciences. Dynamics in such systems typically involves a number of chromophore molecules, for which direct *ab initio* molecular simulations are not computationally feasible. Therefore, developing an efficient way to calculate energies and forces with a minimal sacrifice in accuracy is highly desirable.

This talk summarizes our effort toward studying the energy transfer mechanism in the Fenna-Matthews-Olson (FMO) complex, which has been frequently used as a prototype system for studying photosynthetic energy transfer processes. To elucidate the energy transfer mechanism at a molecular level, we constructed potential energy surfaces of bacteriochlorophyll *a* pigments embedded in the complex by using the potential energy interpolation technique. Our interpolated potential energy surface was then combined with an efficient parallelization algorithm, which enabled us to conduct simulations reaching 100 ns timescales.

By utilizing the speedy nature of our model, we investigated the energetic fluctuations of the pigment molecules in various ways, including the reproduction of the experimental spectral density and the calculation of the solvent response function. We will also briefly show our recent attempts on simulating the nonadiabatic dynamics in the FMO complex, with which we hope to unravel atomistic details of the major energy relaxation channels.

Notes

Excited State Process in Organic Light-emitting Materials

Qian Peng[a], Yuanping Yi[a] and Zhigang Shuai[b,*]

a) Institute of Chemistry, Chinese Academy of Sciences, 100190 Beijing, China.
b) Department of Chemistry, Tsinghua University, 100084 Beijing, China
[*]Email: qpeng@iccas.ac.cn, zgshuai@tisinghua.edu.cn

It is highly desirable to quantitatively predict the luminescence efficiency of large and complicated organic light-emitting materials. Based on Fermi golden rule, we have developed general and analytic formalisms of radiative, internal conversion and intersystem crossing rates using thermal vibration correlation function formula. The displacement, distortion, Duschinsky rotation of potential energy surfaces are taken into account within the multiple harmonic oscillator model, which are necessary to reliably describe the photophysical property of the organic materials. And the luminescent quantum efficiency is evaluated quantitatively from first-principles for the first time. [1]

Applying the formalisms, we have rationalized the exotic aggregation induced emission (AIE) phenomena in organic materials. The AIE mechanism was put forward that the strong emission is recovered by the restriction of the nonradiative decay induced by the electron-vibration coupling in aggregate. Some strategies are proposed to verify the mechanism by using the resonant Raman spectrum, isotopic effect, pressure effect, and the nanoparticle size effect and so on. Some of them have been confirmed by the experiments. Furthermore, the molecular design principles are raised and many unusual AIE fluophors are designed theoretically and synthesized experimentally. [2]

Recently, the long-lived room temperature phosphorescence (RTP) in pure organic system is at the forefront of attention because of its promising application but extremely challenging to achieve highly efficient long-lived RTP materials. Here we present a pair of molecular descriptors to character the phosphorescence efficiency and lifetime. The single-molecular design principle and aggregation-state tuning strategy are proposed by combing extend pi-group and n-group with lone pair electrons, which would balance long lifetime and high efficiency. According to the design principle, many kinds of highly efficient RTP pure organic materials have been synthetized experimentally. [3]

References:

[1] W. Li, L. Zhu, Q. Shi, J. Ren, Q. Peng*, Z. Shuai*, Chem. Phys. Lett. 683, 507 (2017); Z. Shuai*, Q. Peng*, Natl. Sci. Rev. 4, 224 (2017); Z. Shuai*, Q. Peng*, Phys. Reports, 537, 123 (2014); Q. Peng, Y. Niu, Q. Shi, X. Gao, Z. Shuai*, J. Chem. Theory. Comput., 9, 1132 (2013).

[2] T. Zhang, Q. Peng*, C. Quan, H. Nie, Y. Niu, Y. Xie, Z. Zhao, B. Tang, Z. Shuai*, Chem. Sci., 7, 5573 (2016); F. Bu, R. Duan, Y. Xie, Y. Yi, Q. Peng*, R. Hu, A. Qin, Z. Zhao*, B. Tang*, Angew. Chem. Int. Ed., 54, 14492 (2015); T. Zhang, H. Ma, Y. Niu, W. Li, D. Wang, Q. Peng*, Z. Shuai*, W. Liang, J. Phys. Chem. C, 119, 5040 (2015); X. Zheng, Q. Peng*, L. Zhu, Y. Xie, X. Huang*, Z. Shuai*, Nanoscale, 8, 15173(2016).

[3] H. Ma, Q. Peng*, Z. An, W. Huang, Z. Shuai*, J. Am. Chem. Soc., in revision; W. Zhao, Z. He*, Q. Peng*, J. Lam, H. Ma, Z. Qiu, Y. Chen, Z. Zhao, Z. Shuai, Y. Dong*, B. Tang*, Nat. Commun. 9, 3044 (2018); Y. Xiong, Z. Zhao, W. Zhao, H. Ma, Q. Peng, Z. He, X. Zhang, Y. Chen, X. He, J. Lam, B. Tang*, Angew. Chem. Int. Ed. 57, 7997 (2018); Z. He, W. Zhao, J. Lam, Q. Peng*, H. Ma, G. Liang, Z. Shuai, B. Tang*, Nat. Commun., 8, 416 (2017); H. Ma, W. Shi, J. Ren, W. Li, Q. Peng*, Z. Shuai*, J. Phys. Chem. Lett. 7, 2893 (2016).

Notes

Effects of Organic Cation and Electrode Junction on Electronic Structures of $MAPbI_3$

Chang Woo Myung[a], Saqib Javaid[a], Jeonghun Yun[a], Kwang S. Kim[a], and Geunsik Lee[a,*]

a) Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST), Ulsan, 44919, Republic of Korea
[*]Email: gslee@unist.ac.kr

During last five years or so solar cells based on the hybrid perovskite light absorber have shown an enormous improvement up to 22% in the power conversion efficiency. Despites sizable amount of defects inherent in low-cost solution based process, the high efficiency is attributed to a proper size of band gap, high carrier mobility and lifetime, however it is still lacking in detailed microscopic understanding. For further improvement of the hybrid perovskite solar cell efficiency, gaining proper insight would be helpful. Thus electronic structure of $MAPbI_3$ is studied for bulk or interface to an electrode in order to understand the carrier transport or extraction property.

In case of bulk, the vibration of inorganic polar PbI_3 lattice is known to increase the effective mass of electrons via electron-phonon coupling, i.e. formation of Frolich type polaron. However, it is shown here that organic cations embedded in PbI_3 lattice suppress the polaron effective mass via the hydrogen-bond type coupling, so that one can choose a proper type of organic cation towards better mobility [1]. Regarding the carrier lifetime, the Rashba splitting of electronic bands caused by a large spin-orbit coupling of Pb or I and asymmetric shape of MA molecule is known to limit the recombination rate in bulk. We also show that such splitting is enhanced at the interface to TiO_2 or graphene [2]. In case of electrodes, various materials have been investigated to protect a hybrid perovskite against ambient water and to replace commonly used UV-unstable TiO_2, while the band alignment needs to be considered importantly. The band alignment between $MAPbI_3$ and an electrode is also studied for various materials including TiO_2, La-doped $BaSnO_3$ and fluorinated-graphene [3-5].

[1] C. W. Myung, J. Yun, G. Lee, and K. S. Kim, Adv. Energy Mater., **8**, 1702898 (2018).
[2] C. W. Myung, S. Javaid, K. S. Kim, and G. Lee, ACS Energy Lett., **3**, 1294 (2018).
[3] S. Javaid, C. W. Myung, J. Yun, G. Lee, and K. S. Kim, J. Mater. Chem. A, **6**, 4305 (2018).
[4] C. W. Myung, G. Lee, and K. S. Kim, J. Mater. Chem. A, **6**, 23071 (2018).
[5] S. Javaid, C. W. Myung, S. Pourasad, B. Rakshit, K. S. Kim, and G. Lee, J. Mater. Chem. A, **6**, 18635 (2018).

Notes

Generalized Kohn-Sham energy decomposition analysis scheme (GKS-EDA) and its applications

Peifeng Su

The State Key Laboratory of Physical Chemistry of Solid Surfaces, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen, Fujian 361005, China

Email: supi@xmu.edu.cn

The energy decomposition analysis (EDA) schemes bridge the gap between electronic structure theory and conceptually interpretations of intermolecular interactions. The recently developed generalized Kohn-Sham energy decomposition analysis scheme (GKS-EDA),[1] which can perform interaction analysis for open and closed systems in gas phase and solvated environments by various DFT functionals, has been used for various interacting systems, including intramolecular interaction, [2,3] multiple hydrogen bonds,[4] halogen bonds, [5] and so on.

In this talk, the extension of GKS-EDA and its applications for intermolecular interactions with multi-reference characters are provided.

[1] P. Su, Z. Jiang, Z. Chen, W. Wu., *J. Phys. Chem. A,* ***118***, 2531 (2014).
[2] P. Su, Z. Chen, W. Wu. *Chem. Phys. Lett.* **635**, 250 (2015).
[3] P. Su, H. Chen, W. Wu. *Sci. China Chem.* **59**, 1025 (2016).
[4] Z. Liu, C. Trindle, Q. Gu, W. Wu, and P. Su. *Phys. Chem. Chem. Phys.*, **19**, 25260 (2017).
[5] D. Shen, P. Su, W. Wu. *Phys. Chem. Chem. Phys.*, **20**, 26126 (2018)

Notes

List of Participants

Name	Organization	Email
Hiromi Nakai	Waseda University, Japan	nakai@waseda.jp
Jin Yong Lee	Sungkyunkwan University, Korea	jinylee@skku.edu
Weihai Fang	Beijing Normal University, China	fangwh@bnu.edu.cn
Wenjian Liu	Peking University, China	liuwjbdf@gmail.com
Jinlong Yang	University of Science and Technology of China, China	jlyang@ustc.edu.cn
Ganglong Cui	Beijing Normal University, China	ganglong.cui@bnu.edu.cn
Jian Liu	Peking University, China	jianliupku@pku.edu.cn
Linjun Wang	Zhejiang University, China	ljwang@zju.edu.cn
Zhenggang Lan	South China Normal University, China	lanzg@qibebt.ac.cn
Naoki Nakatani	Tokyo Metropolitan University, Japan	naokin@tmu.ac.jp
Ryohei Kishi	Osaka University, Japan	rkishi@cheng.es.osaka-u.ac.jp
Yuki Kurashige	Kyoto University, Japan	kura@kuchem.kyoto-u.ac.jp
Masahiro Higashi	University of the Ryukyus, Japan	higashi@sci.u-ryukyu.ac.jp
Chien-Pin Chou	Waseda University, Japan	cpchou@aoni.waseda.jp
Jae Woo Park	Chungbuk National University, Korea	jaewoopark@cbnu.ac.kr
Chang Woo Kim	Korea Advanced Institute of Science and Technology (KAIST), Korea	cwk91@kaist.ac.kr
Geunsik Lee	Ulsan National Institute of Science and Technology (UNIST), Korea	gslee@unist.ac.kr
Sunkyung Kim	Air Force Academy, Korea	sunkyungkim@afa.ac.kr
Jong-Won Song	Daegu University, Korea	sjoshua@daegu.ac.kr
Zhenyu Li	University of Science and Technology of China, China	zyli@ustc.edu.cn
Igor Ying Zhang	Fudan University, China	igor_zhangying@fudan.edu.cn
Bingbing Suo	Northwest University, China	bsuo@nwu.edu.cn
Lin Shen	Beijing Normal University, China	lshen@bnu.edu.cn
Peifeng Su	Xiamen University, China	supi@xmu.edu.cn
Qian Peng	Institute of Chemsitry, Chinese academy of sciences, China	qpeng@iccas.ac.cn
Ye Mei	East China Normal University, China	samuel.y.mei@gmail.com

Zhendong Li	Beijing Normal University, China	zhendongli2008@gmail.com
Zexing Qu	Jilin University, China	zxqu@jlu.edu.cn
Yingjin Ma	Computer Network Information Center, Chinese Academy of Sciences, China	yingjin.ma@sccas.cn
Chenyang Zhang	Central South University, China	zhangchenyang@csu.edu.cn
Xingyong Wang	University of Wollongong, Australia	xingyong@uow.edu.au
Jinlan Wang	Southeast University, China	jlwang@seu.edu.cn
Yafei Li	Nanjing Normal University, China	liyafei@njnu.edu.cn
Erjun Kan	Nanjing University of Science and Technology, China	ekan@njust.edu.cn
Weijie Hua	Nanjing University of Science and Technology, China	wjhua@njust.edu.cn
Yanan Guo	Nanjing Tech University, China	guoyn@njtech.edu.cn
Yuanjun Gao	Beijing Normal University, China	yuanjun.gao@mail.bnu.edu.cn
Pin Xiao	Beijing Normal University, China	pinxiao@mail.bnu.edu.cn
Zhaoyong Li	Zhejiang University, China	lzypotato@163.com
Cancan Shao	Zhejiang University, China	scc150105@163.com
Shuhua Li	Nanjing University, China	shuhua@nju.edu.cn
Daiqian Xie	Nanjing University, China	dqxie@nju.edu.cn
Jing Ma	Nanjing University, China	majing@nju.edu.cn
Zhaoxu Chen	Nanjing University, China	zxchen@nju.edu.cn
Chungen Liu	Nanjing University, China	cgliu@nju.edu.cn
Haibo Ma	Nanjing University, China	haibo@nju.edu.cn
Wei Li	Nanjing University, China	wli@nju.edu.cn
Yanzi Zhou	Nanjing University, China	zhouyz@nju.edu.cn
Hao Dong	Nanjing University, China	donghao@nju.edu.cn
Shuang Chen	Nanjing University, China	chenshuang@nju.edu.cn
Guixiang Zeng	Nanjing University, China	gxzeng@nju.edu.cn
Chunfeng Zhang	Nanjing University, China	cfzhang@nju.edu.cn
Qingchun Wang	Nanjing University, China	qingchun720@foxmail.com
Zhigang Ni	Nanjing University, China	jsnzg@163.com

Yuqi Wang	Nanjing University, China	mg1724082@smail.nju.edu.cn
Jingxiang Zou	Nanjing University, China	njumath@sina.cn
Wentian Zou	Nanjing University, China	zwtfire@126.com
Dandan Yuan	Nanjing University, China	yddmjm@qq.com
Dongbo Zhao	Nanjing University, China	zdbtwj@163.com
Manyi Yang	Nanjing University, China	ymy0664@163.com
Mingzhou Duan	Nanjing University, China	mingzhou@smail.nju.edu.cn
Zhenxing Li	Nanjing University, China	flyaway333f@163.com
Benkun Hong	Nanjing University, China	qianyeqinfeng@foxmail.com
Shanyu Han	Nanjing University, China	hanshanyu@smail.nju.edu.cn
Feng An	Nanjing University, China	mg1524001@smail.nju.edu.cn
Dongzheng Yang	Nanjing University, China	ydz705@qq.com
Jing Huang	Nanjing University, China	huangj@smail.nju.edu
Junxiang Zuo	Nanjing University, China	jxzuo@smail.nju.edu.cn
Jiaqi Tian	Nanjing University, China	664781314@qq.com
Xinzhu Wang	Nanjing University, China	dz1824035@smail.nju.edu.cn
Ziteng Liu	Nanjing University, China	njuziteng@hotmail.com
Qiang Zhu	Nanjing University, China	csu1505110121@163.com
Yuming Gu	Nanjing University, China	guyuming19930701@163.com
Mengting Fan	Nanjing University, China	1943840935@qq.com
Xiang Li	Nanjing University, China	1014368606@qq.com
Jing Wen	Nanjing University, China	wenjingwinwl@163.com
Harikrishna Sahu	Nanjing University, China	harikrishna@nju.edu.cn
Théophile Gaudin	Nanjing University, China	gaudin.theophile@gmail.com
Xiaoyu Xie	Nanjing University, China	njuxxy2013@gmail.com
Zhen Luo	Nanjing University, China	luozhen07@hotmail.com
Ke Niu	Nanjing University, China	aystwl@126.com
Fangjia Fu	Nanjing University, China	ffj8112991@126.com
Kang Liao	Nanjing University, China	419344228@qq.com
Zheng Cheng	Nanjing University, China	mg1624011@smail.nju.edu.cn

Zheng Wan	Nanjing University, China	2238950918@qq.com
Shirong Wang	Nanjing University, China	wsr@smail.nju.edu.cn
Daibei Yang	Nanjing University, China	151130115@smail.nju.edu.cn
Yuxiao Jin	Nanjing University, China	jinyuxiao@163.com
Zhixing Liu	Nanjing University, China	981120413@qq.com
Yuqin Yang	Nanjing University, China	151070087@smail.nju.edu.cn

誠樸雄偉

勵學敦行