Frontiers in Condensed Matter and Materials Physics:

A Scientific Symposium in Honor of the 75th Birthday of

Steven G. Louie

Physics North Lecture Hall 1, University of California at Berkeley, CA

Saturday, March 2, 2024

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- PROGRAM -

MORNING SESSIONS

Registration and Breakfast (8:00 – 8:30 AM)
Location: Room 375, Physics North Hall.

Welcome Session

8:30-8:40 AM	**Diana Y. Qiu** (Yale University) Introduction Remarks/Logistics
8:40-8:50 AM	**Jeffrey B. Neaton** (University of California, Berkeley, and Lawrence Berkeley National Laboratory) Welcoming Remarks

Note: *All science talks are 15 minutes of presentation + 5 minutes of discussion*

Scientific Session I – ***Two-Dimensional Materials and Moiré Physics***
Chair: Tony F. Heinz (Stanford University)

Location: Room 1, Physics North Hall

8:50-9:10 AM	**Allan H. MacDonald** (University of Texas, Austin) Intra-Band Excitons in Transition-Metal Dichalcogenides Moiré Fractional Chern Insulators
9:10-9:30 AM	**Hyoung Joon Choi** (Yonsei University) Electronic and Phononic Structures of Twisted Transition Metal Dichalcogenides
9:30-9:50 AM	**Feng Wang** (University of California, Berkeley) Explore exciton physics in low dimensional materials
9:50-10:10 AM	**Ting Cao** (University of Washington) New Theoretical Insights into Moiré Solids from Machine Learning

Coffee Break and Symposium Photo (10:10-10:40 AM)
Location: Room 375, Physics North Hall.

Scientific Session II – ***Phonons and Transport Phenomena***
Chair: Matthias Scheffler (Max-Planck-Gesellschaft)

Location: Room 1, Physics North Hall

10:40-11:00 AM	**Feliciano Giustino** (University of Texas, Austin) Self-Trapped Excitons from First Principles, Without Supercells
11:00-11:20 AM	**Cheol-Hwan Park** (Seoul National University) Phonon-assisted optical absorption and phonon-boosted electronic transport

11:20-11:40 AM	**Marina Filip** (Oxford University) Phonon Screening of Excitons in Semiconductors and Insulators
11:40-12:00 PM	**Emmanouil Kioupakis** (University of Michigan) Title: TBD

AFTERNOON SESSIONS

Lunch and Poster Session (12:00-2:00 PM)
Location: Room 375, Physics North Hall.

Scientific Session III – *Strongly Correlated Phenomena*
Chair: Sokrates Pantelides (Vanderbilt University)

Location: Room 1, Physics North Hall

2:00-2:20 PM	**Zhi-Xun Shen** (Stanford University) Surprises from Electron Doped Cuprates: New Insights into Persistent Challenges in High-Temperature Superconductors
2:20-2:40 PM	**Yuanbo Zhang** (Fudan University) Dimensionality-Driven Metal to Mott Insulator Transition in Two-Dimensional 1T-$TaSe_2$
2:40-3:00 PM	**Sangkook Choi** (Korea Institute for Advanced Study) Ab initio Dynamical Mean-Field Theory Methodologies for Correlated Quantum Materials
3:00-3:20 PM	**Xiang Zhang** (The University of Hong Kong) Title: TBD

Coffee Break (3:20-3:50 PM)

Scientific Session IV – *Excitations and Time-Dependent Phenomena*
Chair: Mei-Yin Chou (Academia Sinica)

Location: Room 1, Physics North Hall

3:50-4:10 PM	**Nicola Marzari** (École Polytechnique Fédérale de Lausanne and Paul Scherrer Institut) Spectral Properties from Spectral Functionals
4:10-4:30 PM	**Su Ying Quek** (National University of Singapore) A Journey of Discovery with the Ab Initio GW and GW-Bethe-Salpeter Equation Approaches
4:30-4:50 PM	**Yang-Hao Chan** (Academia Sinica) Time-Dependent Adiabatic GW Approach: Applications and New Developments
4:50-5:10 PM	**Yoshiyuki Miyamoto** (National Institute of Advanced Industrial Science and Technology) Real Time Time-Dependent Density Functional Approach on Defect Dynamics in Diamond Induced by Femtosecond Laser

Closing Remarks

5:10-5:15 PM	**Steven G. Louie** (University of California, Berkeley, and Lawrence Berkeley National Laboratory)

EVENING SESSIONS

Dinner and Short Presentations (6:30-10:00 PM)
Dinner Location: **East Ocean Seafood Restaurant**, 1713 Webster St, Alameda, CA 94501
Shuttle buses will be arranged for transportation.

POSTER TITLES
(Arranged in alphabetical order by authors)

	Presenter and Title
P1	**Timur Bazhirov** (Mat3ra.com) The Digital Ecosystem for Computational Condensed Matter Physics
P2	**Sinisa Coh** (University of California, Riverside) Title: TBD
P3	**Guang-Yu Guo** (National Taiwan University) Title: TBD
P4	**Chen Hu** (University of California, Berkeley) Title: TBD
P5	**Manish Jain** (Indian Institute of Science) Title: TBD
P6	**Leeor Kronik** (Weizmann Institute of Science) Accurate Prediction of Solid-State Electronic and Optical Excitations from Density Functional Theory
P7	**John Lupton** (University of Regensburg) Excitons with Negative-Mass Electrons
P8	**Diana Y. Qiu** (Yale University) Title: TBD
P9	**Jiawei Ruan** (University of California, Berkeley) Title: TBD
P10	**Sufei Shi** (Carnegie Mellon University) Correlated Excitons in Transition-Metal Dichalcogenides Moiré Superlattices
P11	**David Strubbe** (University of California, Merced) New Directions for the Bethe-Salpeter Equation: Spin Flips and Forces
P12	**Liang Z. Tan** (Lawrence Berkeley National Laboratory) Title: TBD
P13	**Johannes Toelle** (California Institute of Technology) GW and Its Connection to Quantum Chemistry
P14	**Wooil Yang** (Korea Institute for Advanced Study) Fully Relativistic First-Principles Calculation with Extended Hubbard Corrections
P15	**Shengbai Zhang** (Rensselaer Polytechnic Institute) Concept of Wigner-Seitz Atom and Solid, and their Application to Band Alignment
P16	**Fangzhou Zhao** (University of California, Santa Barbara, and Max Planck Institute) Trap-Assisted Auger-Meitner Recombination from First Principles
P17	**Zhenfa Zheng** (University of Science and Technology of China and University of Southern California) Ab Initio Real-Time Quantum Dynamics of Charge Carriers in Momentum Space
P18	**Guang-Yu Guo** (*National Taiwan University and National Center for Theoretical Sciences, Taipei, Taiwan*) Nonlinear optical responses and quantum geometry

Abstracts of Invited Talks

Intra-Band Excitons in Transition-Metal Dichalcogenides Moiré Fractional Chern Insulators

Allan H. MacDonald

Department of Physics, University of Texas, Austin

Recent experiments [1, 2] have reported the first observations of fractional Chern insulators (FCIs), exotic states of matter that display a fractional quantum Hall effect in the absence of a magnetic field. The FCIs were discovered in the hole fluids of AA-stacked K-valley transition metal dichalcogenide (TMD) twisted homobilayers. Earlier theoretical work had hinted that FCI states might appear in systems of this type by showing that their moiré minibands could carry Chern numbers [3], that the moiré band width could mysteriously vanish [4] near a magic twist angle, and that the bands have almost ideal quantum geometry [5] when flat. I will explain [6] the appearance of magic angle flat bands and FCIs in these systems by mapping their continuum model to a Landau level problem, and use this framework to discuss intra-valence band collective modes in these systems.

[1] J. Cai *et al.,* Signatures of fractional quantum anomalous hall states in twisted $MoTe_2$, Nature (2023).
[2] Y. Zeng *et al.*, Integer and fractional chern insulators in twisted bilayer $MoTe_2$, Nature (2023).
[3] F. Wu *et al.* Topological insulators in twisted transition metal dichalcogenide homobilayers, Phys. Rev. Lett. **122**, 086402 (2019).
[4] T. Devakul *et al.*, Magic in twisted transition metal dichalcogenide bilayers, Nature Communications **12**, 6730 (2021).
[5] N. Morales-Duran *et al.* Pressure–enhanced fractional chern insulators in moire transition metal dichalcogenides along a magic line, Physical Review Research (2023).
[6] N. Morales-Duran *et al.,* Magic Angles and Fractional Chern Insulators in Twisted Homobilayer TMDs, arXiv: 2308.03143 (2023).

Electronic and Phononic Structures of Twisted Transition Metal Dichalcogenides

Hyoung Joon Choi

Department of Physics, Yonsei University

Twisted multilayers of two-dimensional van der Waals materials are of great interest because of their physical properties that can be tuned by the twist angle. In this study, we report the atomic structures and phononic properties of twisted two-dimensional transition metal dichalcogenides. In particular, we study heterobilayers of $MoSe_2/WSe_2$ monolayers as a function of the twist angle from zero (3R-like) to sixty (2H-like) degrees [1]. Using the Γ-phonon folding model and atomistic calculations, we discuss the twist-angle dependence of the atomic structure relaxation, low-frequency interlayer phonon modes, and high-frequency intralayer phonon modes. We also investigate electronic and optical properties of the 3R- and 2H-like systems using the density functional theory, the GW method, and the Bethe-Salpeter equation. In addition, we discuss phononic properties of twisted monolayer-bilayer systems [2].

[1] S. Y. Lim *et al*., ACS Nano **17**, 13938 (2023).
[2] S. Oh *et al*., 2D Materials **11**, 025004 (2024).

Explore Exciton Physics in Low Dimensional Materials

Feng Wang

Department of Physics, University of California, Berkeley

I will discuss our study of exciton physics with Steve over two decades. I will start with the understanding of exciton in one-dimensional carbon nanotubes, and then continue with the investigation of excitons in two-dimensional transition metal dichalcogenides and moiré heterostructures.

New Theoretical Insights into Moiré Solids from Machine Learning

Ting Cao

Department of Materials Science and Engineering, University of Washington

This talk will show our recent theoretical and computational investigations into moiré superlattices using machine-learning based approaches. We start by demonstrating that a deep neural network guided by first-principles data can be used to examine moiré structural reconstruction in various homobilayers and heterobilayers of transition metal dichalcogenides. Going beyond the capacity of direct DFT calculations, our machine-learning enabled workflow discovers salient structural features and key topological characters controlled by twist angles, layer composition, and other tuning knobs. This knowledge can be used to inform accurate continuum models, and to predict new forms of moiré potential and moiré topology. Finally, we connect our theoretical discoveries to experimental results and explore potential applications.

Scientific Session II – *Phonons and Transport Phenomena*

Self-Trapped Excitons from First Principles, without Supercells

Feliciano Giustino

Department of Physics and Oden Institute, University of Texas, Austin

Excitons are composite quasiparticles formed when an electron and a hole in a crystal bind together under the effect of their attractive Coulomb interaction. In some materials, the spatial fluctuations of the electric charge density of the exciton polarizes the surrounding crystal lattice, and in turn this distortion promotes the spatial localization of the exciton. This feedback loop between exciton and crystal lattice leads to a new type of quasiparticle called excitonic polaron. In materials with strong exciton-phonon couplings, these quasiparticles are unable to diffuse and become self-trapped excitons. First-principles calculations of excitonic polarons and self-trapped excitons are challenging because they require large supercells involving hundreds or thousands of atoms. In this talk, I will discuss a new methodology that combines density-functional perturbation theory and the Bethe-Salpeter approach to compute excitonic polarons and self-trapped excitons from first principles, without resorting to supercell calculations [1,2]. This method generalizes the ab initio theory of polarons developed by our group [3-7] to the case of excitonic quasiparticles. I will illustrate this methodology by discussing exciton-phonon interactions and excitonic polarons in alkali halides and halide perovskites.

[1] Z. Dai, C. Lian, J. Lafuente-Bartolomé, and F. Giustino, “Excitonic polarons and self-trapped excitons from first-principles exciton-phonon couplings”, Phys. Rev. Lett. **132**, 036902 (2024).
[2] Z. Dai, C. Lian, J. Lafuente-Bartolomé, and F. Giustino, “Theory of excitonic polarons: From models to first-principles calculations”, Phys. Rev. B **109**, 045202 (2024).
[3] W. H. Sio, C. Verdi, S. Poncé, and F. Giustino, “Polarons from first principles, without supercells”, Phys. Rev. Lett. **122**, 246403 (2019).
[4] W. H. Sio, C. Verdi, S. Poncé, and F. Giustino, “Ab initio theory of polarons: Formalism and applications”, Phys. Rev. B **99**, 235139 (2019).
[5] J. Lafuente-Bartolomé, C. Lian, W. H. Sio, I. G. Gurtubay, A. Eiguren, and F. Giustino, “Ab initio self-consistent many-body theory of polarons at all couplings”, Phys. Rev. B **106**, 075119 (2022).
[6] J. Lafuente-Bartolomé, C. Lian, W. H. Sio, I. G. Gurtubay, A. Eiguren, and F. Giustino, “Unified approach to polarons and phonon-induced band structure renormalization”, Phys. Rev. Lett. **129**, 076402 (2022).
[7] W.-H. Sio and F. Giustino, “Polarons in two-dimensional atomic crystals”, Nat. Phys. **19**, 629 (2023).

Phonon-Assisted Optical Absorption and Phonon-Boosted Electronic Transport

Cheol-Hwan Park

Department of Physics, Seoul National University

In this presentation, I will first discuss a method to describe the phonon-assisted optical absorption from first principles that can describe both the phonon-induced bandstructure renormalization and the difference between phonon absorption and emission processes properly [1]. Then, I will discuss some particular electronic transport that can be boosted by electron-phonon interactions [2].

[1] J.-M. Lihm and C.-H. Park, Phys. Rev. X **11**, 041053 (2021).
[2] J.-M. Lihm and C.-H. Park, unpublished.

Phonon screening of excitons in semiconductors and insulators

Marina R. Filip

Department of Physics, University of Oxford

Understanding the physics of how excitons form, delocalize and dissociate is of key importance to the functionality of a wide range of applications, such as photovoltaics, lighting and lasing. Development of new computational modeling techniques based on density functional theory (DFT) and many body perturbation theory capable to describe interactions between excitons and other quasiparticles constitutes a frontier first principles computational modeling of materials. The GW+Bethe-Salpeter Equation (BSE) approach [1,2] is the state-of-the-art approach to compute optical excitation energies in semiconductors and insulators and provides the foundation of new methods aimed at describing complex excited state phenomena. In this talk, I will present a new development that allows us to understand from first principles the impact of ionic vibrations have on the dielectric screening of excitons [3,4]. I will first present the main theoretical approach, and show how this allows us to compute temperature dependent exciton binding energies, as well the rate of dissociation of excitons upon scattering with phonons from first principles [4,5]. Secondly, I will present a set of results we obtained by applying this approach to several well known semiconductors and insulators, and compared to experimental data available in the literature.

[1] Hybertsen & Louie, Phys. Rev. B **34**, 5390 (1986).
[2] Rohlfing & Louie, Phys. Rev. Lett. **81**, 2312 (1998).
[3] Filip, Haber & Neaton, Phys. Rev. Lett. **127**, 67401 (2021).
[4] Alvertis, Haber, Li, Coveney, Louie, Filip & Neaton, submitted (2023), arXiv:2312.03841.
[5] Coveney, Haber, Alvertis, Neaton & Filip, submitted (2023).

Scientific Session II – *Phonons and Transport Phenomena*

Title: TBD

Emmanouil Kioupakis

Department of Materials Science and Engineering, University of Michigan

Abstract: TBD.

Surprises from Electron Doped Cuprates: New Insights into Persistent Challenges in High-Temperature Superconductors

Zhi-Xun Shen

Departments of Physics and Applied Physics, Stanford Institute for Materials and Energy Sciences, Stanford University

The enigma of high-temperature superconductivity in copper oxides, defying the predictions of BCS theory with its unexpectedly high critical temperature, persists as a captivating yet unresolved physics problem. The complexity lies in its seemingly paradoxical nature—simple as a single-band and ½ spin system, yet remarkably intricate, exhibiting d-wave superconductivity, pseudogap, spin and charge orders, and peculiar phenomena associated with strange metals. Cuprates, in this context, epitomize the intellectual challenge posed by correlated electrons, sparking discussions ranging from the physics of the Hubbard model and quantum critical point to Planckian metal, influencing conversations across diverse topics, from cold atoms to twist-stacked 2D materials.

While much attention in cuprate research has historically focused on the hole-doped side, the electron-doped side has received less scrutiny, likely due to its lower transition temperature. In this presentation, I explore recent revelations in the electronic phase diagram of n-type cuprates, unearthing surprises that reshape our understanding: i) The presence of Bogoliubov quasiparticles on a delicate gossamer Fermi surface—challenging the conventional notion that superconductivity maximizes on the antiferromagnetically reconstructed Fermi surface, instead occurring at the antiferromagnetic "hot spot," where the Fermi surface is maximally gapped by the antiferromagnetic pseudogap [1]; ii) Unearthing an anomalous normal state gap—revealing that the perceived antiferromagnetic metal in the underdoped regime, with a reconstructed Fermi surface and long-range antiferromagnetic order, is further gapped by effects extending beyond antiferromagnetism. Considering all known ordering tendencies alongside the phase diagram, we hypothesize that this gap originates from Cooper pairing at a much higher temperature scale than previously believed [2].

These discoveries are discussed against the backdrop of persistent challenges in the cuprate problem: a) The elusive origin of the pseudogap; b) The intricate dance of electrons in a single band, navigating the competing demands of "to pair" and "to be paired"; c) The interplay of competing orders. As we delve into these complexities, the intricate dance of electrons in copper oxides unfolds, revealing layers of mystery that continue to captivate and challenge our understanding of condensed matter physics.

[1] Ke-Jun Xu, Qinda Guo, Makoto Hashimoto, Zi-Xiang Li, S.D. Chen, J.F. He, Yu He, Gong Li, M.H. Berntsen, C.R. Rotundu, Y.S. Lee, T.P. Devereaux, A. Rydh, D.H. Lu, D.H. Lee, O. Tjernberg, Z.-X. Shen, Nature Physics **19** (12), 1834-1840 (2023).
[2] Ke-Jun Xu, J.F. He, S. Abadi, S.D. Chen, Yu He, C.R. Rotundu, Y.S. Lee, D.H. Lu, Qinda Quo, O. Tjernberg, T. P. Devereaux, D.H. Lee, M. Hashimoto, Z.-X. Shen, under review.

Dimensionality-Driven Metal to Mott Insulator Transition in Two-Dimensional 1T-$TaSe_2$

Yuanbo Zhang

Departments of Physics, Fudan University

Two-dimensional materials represent a major frontier for research into exotic many-body quantum phenomena. In the extreme two-dimensional limit, electron-electron interaction often dominates over other electronic energy scales, leading to strongly correlated effects such as quantum spin liquid and unconventional superconductivity. The dominance is conventionally attributed to the lack of electron screening in the third dimension. In this talk, I will describe our recent finding of an intriguing metal to Mott insulator transition in 1T-$TaSe_2$ that defies the conventional wisdom. Specifically, we find that dimensionality crossover, instead of reduced screening, drives the transition in atomically thin 1T-$TaSe_2$. A dispersive band crossing Fermi level is found to be responsible for the bulk metallicity in the material. Reducing the dimensionality, however, effectively quenches the kinetic energy of these initially itinerant electrons, and drives the material into a Mott insulating state. The dimensionality-driven Metal to Mott insulator transition resolves the long-standing dichotomy between metallic bulk and insulating surface of 1T-$TaSe_2$, and introduces a novel approach to modulating the electronic structure of two-dimensional materials.

Ab Initio Dynamical Mean-Field Theory Methodologies for Correlated Quantum Materials

Sangkook Choi

School of Computational Sciences, Korea Institute for Advanced Study

Quantum information science is a surging frontier of physical science. By creating quantum states and utilizing them as quantum bits (qubits), it promises vastly improved performance over what we have achieved during the 20th century. Quantum materials are a class of materials of which properties can be explained by only quantum physics. When their quantum nature is due to electron-electron interaction, quantum materials give rise to a rich tableau of novel physics. These so-called correlated quantum materials can be utilized as “semiconductors” for quantum information science. However, understanding correlated quantum materials properties is one of the grand challenges in the field of quantum materials. Correlated quantum materials preclude simple explanations and computationally simple methods based on Landau’s Fermi liquid theory, such as density functional theory. In this talk, I'll introduce ab initio DMFT approaches, especially LQSGW+DMFT[1,2] and full GW+EDMFT [3] . I will also show several interesting physics found in correlated quantum material including infinite-layer nickelate [4,5], Fe-based superconductors [6].

[1] S. Choi, P. Semon, B. Kang, A. Kutepov, and G. Kotliar, Comp. Phys. Comm. **244**, 277 (2019)
[2] S. Choi, A. Kutepov, K. Haule, M. van Schilfgaarde, and G. Kotliar, npj Quantum Materials **1**, 16001 (2016)
[3] B. Kang, P. Semon, C. Melnick, G. Kotliar, and S. Choi, arXiv:2310.04613.
[4] S. Ryee, P. Semon, M. J. Han, and S. Choi, Phys. Rev. Lett. **126**, 206401 (2021)
[5] B. Kang, C. Melnick, P. Semon, S. Ryee, M. J. Han, G. Kotliar, and S. Choi, npj Quantum Mater. **8**, 1 (2023)
[6] M. Kim, S. Choi, W. H. Brito, and G. Kotliar, arXiv:2304.05002.

Scientific Session III – *Strongly Correlated Phenomena*

Title: TBD

Xiang Zhang

Faculty of Science, The University of Hong Kong

Abstract: TBD.

Spectral Properties from Spectral Functionals

Nicola Marzari

École Polytechnique Fédérale de Lausanne and Paul Scherrer Institut

I discuss the development of functional theories to describe charged excitation (ionization potentials, electron affinities, band structures) and spectral properties, developing functional theories of the spectral density, and their quasiparticle approximation in the form of orbital-density dependent Koopmans functionals.

Work done in collaboration with Nicola Colonna, Edward Linscott, and the authors of [1], and with Andrea Ferretti, Tommaso Chiarotti, Mario Caserta, and Alessandro Carbone [2].

[1] Edward B. Linscott, Nicola Colonna, Riccardo De Gennaro, Ngoc Linh Nguyen, Giovanni Borghi, Andrea Ferretti. Ismaila Dabo, Nicola Marzari, J. Chem. Theory Comput., **19**, 20, 7097–7111 (2023).
[2] Tommaso Chiarotti, Andrea Ferretti, and Nicola Marzari, https://arxiv.org/abs/2302.12193 (2023).

A Journey of Discovery with the Ab Initio GW and GW-Bethe-Salpeter Equation Approaches

Su Ying Quek

Department of Physics and Centre for Advanced 2D Materials, National University of Singapore

Professor Steven G. Louie, and his students and post-docs, were among the pioneers of the *ab initio* GW [1], and GW-Bethe-Salpeter Equation (BSE) approaches [2], with recent developments in enhancing the accuracy of these approaches for 2D materials [3]. In this talk, I will share how these approaches have played a key role in my journey of scientific discovery, that I have been fortunate to embark on with several talented group members. Starting off with an interest in energy level alignment stemming from my time in Berkeley with Jeff Neaton and Professor Louie, we developed approaches to accelerate GW calculations for interfaces in large supercells, and demonstrated analytically and numerically the validity of these approximations in different cases [4]. With GW-BSE calculations, we further predicted the possibility of high temperature Bose-Einstein condensation of excitons in organic-2D material systems [5]. We were also interested in quantifying the Landé g-factors and associated Landau levels within the GW approximation [6]; we developed approaches to treat both static and dynamical self-energy effects on the g-factors, and demonstrated significant enhancement in the g-factors in doped materials [7]. Finally, we studied non-linear optical responses within the GW-BSE approximation [8]; we provide physically compelling reasons to show that excitons should in general enhance the non-linear optical response, define a shift vector in the many-body picture, and demonstrate the importance of excitonic resonances and inter-exciton transitions in spontaneous parametric down conversion/sum frequency generation. Throughout this journey, we have found that these approaches provide very reasonable agreement with benchmark experiments, demonstrating that Professor Louie's legacy in ab initio GW and GW-BSE approaches enables predictions in new realms of science.

[1] PRB **34**, 5390 (1986); [2] PRB **62**, 4927 (2020); [3] PRB **95**, 035109 (2017); [4] JCTC **15**, 3824 (2019), JPCL **11**, 9358 (2020), JPCL **12**, 8841 (2021), npj 2D materials and applications, **6**, 73 (2022); [5] Nano Lett, **21**, 8888 (2021); [6] Physical Review Research, **2**, 033256 (2020); [7] npj Computational Materials, **7**, 198 (2021); [8] arXiv:2305.08345, arXiv:2402.02002

Time-Dependent Adiabatic GW Approach: Applications and New Developments

Yang-Hao Chan

Institute of Atomic and Molecular Sciences, Academia Sinica
National Center of Theoretical Sciences, Physics Division

The real-time, non-equilibrium Green function method within the adiabatic GW approximation (TD-aGW) has been applied to atomically thin quasi-2D insulating materials to exhibit novel exciton physics, such as excitonic shift current and exciton-Floquet phenomena. It has also been applied to study excitonic effects on second harmonic generation, high harmonic generation, and ultrafast charge transfer in MoS2/WS2 heterostructure. In this presentation, we would like to demonstrate some of the applications and discuss our recent development on including electron-phonon couplings. In particular, we will show that excitonic effects in the IR and Raman spectroscopy can be described, based on a perturbative expansion of both electron-phonon and electron-light couplings in the TD-aGW framework.

Scientific Session IV – *Excitations and Time-Dependent Phenomena*

Real Time Time-Dependent Density Functional Approach on Defect Dynamics in Diamond Induced by Femtosecond Laser

Yoshiyuki Miyamoto

National Institute of Advanced Industrial Science and Technology

In this presentation, I will discuss computational analysis of recent experimental report to form nitrogen-vacancy (NV) center in diamond by using single beam of the femtosecond laser. As NV center has become potential quantum device using its long spin-coherent time as well as light emission, an efficient way of formation of the NV center in diamond has become crucial for practical applications. Since controlling crystalline quality of diamond as well as impurity doping need high-temperature process around 1000 degrees, fabrication of diamond devices is challenging due to risks of thermal damage of surrounding materials.

Advent of femtosecond laser enabled us to curry out non-thermal process using electronic excitation, and recent experiment by Fujiwara et al., [https://doi.org/10.1063/5.0137093] demonstrated formation of NV center using single laser irradiation with duration time of 35 fs and wavelength of 810 nm. Meanwhile, previous theoretical work by Kempkes et al., [https://doi.org/10.1016/j.carbon.2020.12.062] reported vacancy diffusion to form NV center in diamond under assumption of thermalized electrons, but this work cannot be directly compared with the experimental laser condition.

In this talk, I will present the real-time time-dependent density functional approach coupled with ion dynamics within the Ehrenfest approximation and demonstrate vacancy diffusion toward nearest site of a nitrogen (N) impurity in diamond with presence of laser field. When a vacancy initially locates at the second nearest site of the N impurity, barrier-less vacancy diffusion upon laser irradiation was observed. More complicated conditions like as farther location of the vacancy from the N impurity or dynamics without vacancy will also be discussed.

This work was performed under support by MEXT Quantum Leap Flagship Program (MEXT Q-LEAP) Grant Number JPMXS0118067395.