Interdisciplinary symposium on modern density functional theory

Monday 19 June 2017 - Friday 23 June 2017

Okochi Hall, RIKEN (Wako campus)

Book of abstracts

Describing Quantum Phases of Matter and their Dynamics within Density Functional Theory and Time-Dependent Density Functional Theory

Monday 19 June 2017 09:30
Presenter: Prof. GROSS, E.K.U. (Max Planck Institute of Microstructure Physics)

After an overview of the basic concepts of standard ground-state density functional theory (DFT) as well as time-dependent DFT (TDDFT), the description of quantum phases, such as magnetism and superconductivity will be addressed within this framework. The idea is to include the order parameter describing the respective phases explicitly [1,2] in the exchange-correlation functional of DFT/TDDFT. As a real-world example, the laser-induced demagnetization of ferromagnets [3] and the ultrafast magnetization transfer between sublattices of some Heusler compounds [4] will be calculated by real-time TDDFT. Furthermore, some thoughts will be presented on how to tackle topological phases of matter in a DFT/TDDFT framework [5], exemplified by the Berry phase [6] associated with the Beyond-Born-Oppenheimer description [7] of molecular motion.

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The role of tensor force in heavy-ion fusion dynamics

Monday 19 June 2017 11:15
Presenter: Dr. GUO, Lu (University of CAS)

The tensor interaction is of current interests in nuclear physics. It could play a major role in structure, in particular away from stability, as well as in reaction. We systematically investigate the effect of tensor force on the fusion cross-section and Coulomb barrier in heavy-ion fusion dynamics within the symmetry-unrestricted three-dimensional time-dependent Hartree-Fock (TDHF) theory. The full version of Skyrme interaction, including the terms from the tensor force, is incorporated in our TDHF implementation. We found that the Coulomb barrier is systematically increased by the inclusion of tensor force for the spin-unsaturated systems, and has better agreement with the experiments than those without the tensor force included. A notable effect for the fusion cross-section is observed in the spin-unsaturated systems, and its agreement with experiments is significantly improved by the inclusion of tensor force. These effects of tensor force in fusion dynamics is attributed to the shift of low-lying vibration states with the inclusion of tensor force.

Linear Scaling Solvers for Density Functional Theory Calculations

Monday 19 June 2017 11:45
Presenter: Dr. DAWSON, William (RIKEN)

The theory of matrix functions is a well developed framework with a wide range of applications including differential equations, graph theory, and electronic structure calculations. One particularly important application area is diagonalization free methods in density functional theory calculations. When the input and output of the matrix function are sparse, methods based on polynomial expansions can be used to compute matrix functions in linear time. In this talk, we present a library based on these methods that can compute a variety of matrix functions. We will describe the algorithms at the heart of this library, and show how can be integrated into a variety of programs to enable large scale calculations.

Low-order scaling methods in density functional theories

Monday 19 June 2017 13:30
Presenter: Prof. OZAKI, Taisuke (ISSP, Univ. of Tokyo)

Density functional theories (DFT) have been widely used in chemistry and condensed matter physics, and proven to be a versatile theoretical tool in predicting electronic and geometrical properties of molecules and solids. Having the success of DFT in mind, a next challenge is to simulate more realistic systems involving complex interface structures such as Li ion batteries, permanent magnets, and structural materials, for which the interfaces and grain boundaries play a crucial role in determining the performance of devices. Computational models for these systems may consist of several thousand atoms at least, and oversimplified models may lose fundamental physical processes determining the performance of devices. However, such a simulation tends to be hampered by the computational complexity of DFT calculations which intrinsically scales as O(N3), where N is the number of atoms in the system under investigation.

Here, we report our development of low-order scaling methods in DFT based on quantum nearsightedness of electron, whose computational scaling is lower than the cube of the number of atoms N [1-5,13], towards realistic large-scale simulations. An approximate O(N) method based on a Krylov subspace technique [2] and a numerimcally exact low-order scaling method [4] will be introduced in details together with illustrative applications [8-12]. It will be also shown that the idea based on the quantum nearsightedness can be applied to developments of an O(N) non-equibrium Green's function (NEGF) method and a nearly exact exchange functional [5]. Furthermore, a novel parallelization method has been developed based on an inertia tensor moment method to realize large-scale DFT calculations on massively parallel computers typified by the K-computer [6,7].

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Covariant density functional theory for nuclear structure

Monday 19 June 2017 15:15
Presenter: Prof. MENG, Jie (Peking University)

Covariant density functional theory with a minimal number of parameters allows a very successful description of nuclear structure properties range from ground state to excited state all over the nuclear chart. With pairing correlations and the continuum effect properly taken into account, the self-consistent microscopic descriptions and predictions of the neutron halo phenomena in both spherical and deformed nuclei become possible. Constrained and cranking calculations, CDFT in a static external field, are powerful tools to investigate the shape evolution, shape isomers, shape-coexistence, fission landscapes, and rotational spectra in both near spherical and deformed nuclei. RPA calculation based on CDFT provides a successful description of the mean energies of nuclear giant resonances. The restoration of symmetries and configuration mixing to take into account fluctuations around the mean-field equilibrium based on CDFT as well as its simplification, collective Hamiltonian, describe well the nuclear low-lying states and shape transitions well. Future perspective on CDFT application for nuclear astrophysics and its future development will be discussed.

Exact time-dependent Kohn-Sham potentials in electron-scattering processes

Monday 19 June 2017 16:30
Presenter: Dr. SUZUKI, Yasumitsu (Tokyo University of Science)

Time-dependent density functional theory (TDDFT) is one of the most useful first-principles approaches to study the real-time many-body electron dynamics. However, the validity of its application to the electron-scattering processes has not been clear because of the lack of knowledge whether the current available exchange-correlation (XC) functional is reliable for such situations. In this study we have computed the exact time-dependent Kohn-Sham potential in the one-dimensional two-electron scattering system that models electron - hydrogen scattering. We will present the analysis of them and the idea how to refine their approximation.

Maxwell+TDDFT multiscale method for light-matter interaction: light propagation in the microscopic semiconducting crystal

Monday 19 June 2017 16:45
Presenter: Mr. UEMOTO, Mitsuharu (University of Tsukuba)

Due to the rapid growth of the computing resources, the large-scale simulation of the light matter interaction between the microscopic objects and intense light field becomes possible. The first principle time-dependent density functional theory (TDDFT) is a powerful tool to compute the optical properties of solids in the intense electric field. On the other hand, the finite-difference time-domain (FDTD) is also well used to solve the electromagnetic field problems by the microscopic materials. In this work, we have been developing the Maxwell+TDDFT multiscale technique combining the TDDFT and FDTD method to treat propagation and scattering of the intense laser pulses. In our approach, the light field is calculated by the FDTD-like formalism defined on the macroscopic grid. At each macroscopic point, the TDDFT based electron dynamics calculation is employed. At this time, we will introduce the demonstration of this method to problems that require 1D, 2D, and 3D description for light propagations.

Finite amplitude method for triaxially deformed superfluid nuclei

Monday 19 June 2017 17:00
Presenter: Dr. WASHIYAMA, Kouhei (Center for Computational Sciences, University of Tsukuba)

Our goal is to construct a microscopic quadrupole collective Hamiltonian model to treat large-amplitude shape fluctuation and shape mixing in nuclei. This model consists of the constrained density functional theory (Hartree-Fock-Bogoliubov) and local quasiparticle random phase approximation (LQRPA) based on DFT with Skyrme functionals. Since QRPA calculations for deformed nuclei require large resources of computations, QRPA for triaxially deformed nuclei is currently not available. The finite amplitude method (FAM) was proposed [1], and then has been applied to wide range of nuclei [2-5]. Main advantages of FAM are that functional derivative of Hamiltonian as the residual interactions, which requires large computations, is replaced with a finite-difference form, and construction and diagonalization of huge QRPA matrices are avoided by using an iterative method. These two advantages considerably reduce the computational cost for performing QRPA calculations, especially for deformed nuclei.

As a first step to construct the microscopic collective Hamiltonian mentioned above, we develop a computer code of FAM QRPA for triaxial nuclei with the full Skyrme energy density functionals. In this contribution, we will present results of multipole strength functions and sum rules of triaxial nuclei such as 110Ru.

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Effect of Stacking Interactions and Conformation on Polymer Polarizability

Monday 19 June 2017 17:15
Presenter: Dr. MOORTHI, Krzysztof (Mitsui Chemicals, Inc.)

The Long-Range Corrected density functionals (LC-DF)[1] represent dynamical polarizabilities of medium-sized organic and metal-organic compounds with very good accuracy.[4,5] The functional with 100% of Hartree–Fock (HF) exchange at long-range, LC-BLYP[2], performs best for aromatic compounds and CAM-B3LYP[3] for saturated compounds. These excellent benchmark results motivated us to apply LC-DF's to study optical properties of polymers.
If repeat unit models are corrected for end-effects, refractive index and Abbe number of large number of non-conjugated polymers is represented with very good accuracy, for example, for polystyrene (PS), poly(methyl methacrylate) and CYTOP wavelength-dependent refractive indices exceptionally good agreement (rmsd within 0.004).[6] The latter results, as well as some tendency to overestimate refractive index in polymers rich in large aromatic moieties, prompted us to study how stacking between aromatic moieties affects polarizability.[7] We study diads (dimers) with aromatic substituents containing six to fourteen pi electrons. The stacking of aromatic substituents in meso-tg, racemo-tg and racemo-tt conformers causes polarizability decrease relative to conformers, in which substituents are separated, for example, meso-tg. The polarizability reduction is more pronounced in larger aromatic systems. In PS, the experiment [8] and simulations [9] suggest that meso-tg, racemo-tg and racemo-tt diads are favored, in which no stacking of phenylenes is observed. Consequently, the refractive index based on (simulated and experimental) diad populations, is practically the same as the monomer-based refractive index, with both values in excellent agreement with the experimental value of 1.592.[6] We extend this analysis to, among others, poly(ethylene terephthalate), for which a nonbonded dimer model similar to that of parallel displaced benzene dimer predicts refractive index in excellent agreement with experiment. From the knowledge of polarizability changes upon stacking, and conformer population, estimation of this effect in condensed systems appears possible.

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Basics of electron structure DFT in chemistry, condensed-matter, and materials science: From the very fundamental to the very latest (machine-learning)

Tuesday 20 June 2017 09:30
Presenter: Prof. BURKE, Kieron (UC Irvine)

In the first half of my talk, I will explain how DFT has become the standard method for performing electronic structure calculations in many fields, with over 30,000 papers applying DFT each year[1,2]. In the second half, I will discuss some very recent results from very different approaches: The semiclassical origins of DFT[3], and functionals found by machines[4,5].

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Large-Scale First-Principles Electronic Structure Calculations in Petascale and Exascale Supercomputers: A Real-Space Density Functional Theory code

Tuesday 20 June 2017 11:15
Presenter: Dr. IWATA, Junichi (Department of Applied Physics, The University of Tokyo)

First-principles electronic structure calculation based on the Density Functional Theory (DFT) has been an indispensable tool for many fields of material science and engineering. With the development of supercomputers, the target size of a first-principles DFT calculation becomes larger and larger, and nowadays, a few hundreds to a thousand of atoms has been computable with standard plane-wave based DFT program codes. However, the computable sizes are still not satisfactory for clarifying or designing the material properties in realistic situations. The challenge for large scale calculations with state-of-the-art supercomputers is one of the ways to overcome the size difficulty in the first-principles electronic structure calculations.

In this talk, I'd like to introduce our program code RSDFT [1], which has been developed to perform large-scale first-principles calculations on massively-parallel computers including the Japanese flagship machine K computer [2]. RSDFT is based on the real-space finite-difference pseudopotential method. Contrary to the standard plane-wave methods, the real-space method needs not to use Fast Fourier Transformations, which requires heavy communication burden, and therefore the scalability of RSDFT is rather good even in the calculations with tens of thousands of compute nodes [3]. It has also been started to develop RSDFT for the next flagship computer called post-K computer, and we aim to make first-principles calculations on the system with a few thousand of atoms easy tasks. I would like to also talk about the development of RSDFT for the post-K computer.

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Covariant density functional theory with Fock terms—role of the non-local Fock terms

Tuesday 20 June 2017 11:45
Presenter: Prof. LONG, Wenhui

In this talk, I will briefly introduce the covariant density functional theory with Fock terms. Firstly I will briefly introduce the theory itself, including the backgound, history, and theoretical framework. Then the discussions will be concentrated on the role of Fock terms in nuclear structure, including the balance of nuclear force, the prediction of novel phenomena, and the nuclear tensor force. Finally, a short conclusion and perspective will be given.

DFT versus many-body perturbation theory for nuclear structure

Tuesday 20 June 2017 13:30
Presenter: Prof. COLO, Gianluca (University of Milano/INFN)

The applicability of Density Functional Theory to the nuclear case, its many successes and the open problems, are a vast domain. In this contribution, I will mainly focus on two questions.

First, I will discuss how to obtain realistic values for the bulk nuclear properties, either within the Hartree-Fock or Kohn-Sham scheme. It will be argued that, so far, only the Kohn-Sham scheme has been able to produce nuclear saturation and reasonable nuclear binding energies without too much of a tension with the rest of the nuclear phenomenology, in particular with the single-particle properties and the nucleon effective mass.

Yet, many experimental findings are not explained within Kohn-Sham DFT. I will introduce the Green's function methods for nuclear structure, in particular along the idea of particle-vibration coupling (PVC). The rationale behind it, is that the low-lying spectra of nuclei are indeed governed by the interplay between single-particle and vibrational degrees of freedom. I will show applications to giant resonances, charge-exchange transitions and low-lying states in odd-nuclei. I will try to draw analogies with, e.g., the GW-method for electronic systems; more generally, I will advocate the need of a stronger cross-fertilizations between the study of nucleonic and electronic systems.

Improving usability of DFT codes by using GUI software C-Tools

Tuesday 20 June 2017 15:15
Presenter: Dr. YOSHIZAWA, Kanako (Research Organization for Information Science & Technology)

We develop GUI software C-Tools [1] to improve the usability of DFT codes for materials. There are a variety of DFT codes with each strength, and to combine the strength we have to transfer among the codes. For this purpose, we have developed an input format conversion system, named as C-Tools, with a developed unified input format in XML as a common interlanguage among various formats. C-Tools can convert the input files between different codes and can generate an input file from a structure file for a material. The input files can be easily created by clicking the [load] and [save] button. Now C-Tools supports the five file formats for DFT codes, xTAPP [2], OpenMX [3], RSDFT [4], VASP [5], and Quantum ESPRESSO (PWscf) [6]. We can use C-Tools for performance analysis of DFT codes in HPCI system. We show the results in K computer.

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A novel method to predict densities of amorphous materials from first-principles calculations

Tuesday 20 June 2017 15:30
Presenter: Mr. FURUKAWA, Yoritaka (The Univesity of Tokyo)

First-principles calculations had not ever been performed to predict the densities of amorphous materials. This was due to the fact that because of the disordered nature of amorphous materials, their atomic configurations are completely different from one sample to another, and thus there is no one-to-one correspondence between the densities and the total energies. In our study, to remedy this problem, we have devised a novel method which employs the density functional theory (DFT) and the Car-Parrinello molecular dynamics method based on the DFT. We have applied it to amorphous silicon and found that the determined density and its bulk modulus are in good agreement with experiment. The results suggest the validity of the proposed method.

Spin and Spin-isospin responses in N=Z nuclei and Isoscalar pairing correlations

Tuesday 20 June 2017 15:45
Presenter: Prof. SAGAWA, HIROYUKI (RIKEN/UNIVERSITY OF AIZU)

The spin magnetic dipole transitions and the neutron-proton spin-spin correlations in $sd-$shell even-even nuclei with $N=Z$ are investigated using shell model wave functions. The isoscalar (IS) spin-triplet pairing correlation provides a substantial quenching effect on the spin magnetic dipole transitions, especially on the isovector (IV) ones.
Consequently, an enhanced isoscalar spin-triplet pairing interaction influences the proton-neutron spin-spin correlation deduced from the difference between the IS and the IV sum rule strengths. The effects of the higher configuration mixings, exchange currents and $\Delta(\Delta(33)$ resonance)-hole coupling are also examined in the spin transitions and the spin-spin correlations of the ground states.

Spin-isospin responses in low-energy

Tuesday 20 June 2017 16:00
Presenter: Dr. YOSHIDA, Kenichi (Kyoto University)

Excitation modes associated with both spin and isospin degrees of freedom are unique in nuclear system. I am going to focus on the low-frequeny modes of excitation that can have an impact on the beta-decay rate.

Tensor effects on the isospin excitation with random phase approximation based on relativistic Hartree-Fock approach

Tuesday 20 June 2017 16:15
Presenter: Mr. WANG, Zhiheng (Center for Computational Sciences, University of Tsukuba)

The relativistic representation of the nuclear tensor force has been developed recently. In order to investigate the effects of the tensor force on the isospin excitation in a covariant way, we added the contributions of ρ-tensor couplings to the existing random phase approximation (RPA) based on the relativistic Hartree-Fock approach (RHF). As the first step to study the effects of the tensor force, we will present some results of the RHF+RPA using the parameter set PKA1 and discuss the possible effects of the ρ-tensor couplings. And the plan for the future work will be given.

Band unfolding calculations compared with ARPES experiments: Examples of Ni1/3TiS2 and twisted-bilayer graphene

Tuesday 20 June 2017 16:30
Presenter: Dr. MATSUSHITA, Yu-ichiro (The University of Tokyo)

Electronic band structure calculations based on the density-functional theory (DFT) collaborating with Angle-Resolved-Photo-Emission Spectroscopy (ARPES) measurements is a very powerful tool to investigate the electronic properties of condensed matters. However, we often face a big problem of the “band folding”, when we use the supercell scheme. The folded and “dense” electronic bands in the supercell Brillouin zone are not similar to the experimentally obtained band structures by ARPES anymore, which makes it difficult to compare them directly.

Recently band unfolding method was proposed and used for many systems. In our recent studies, we applied the band unfolding method to Ni1/3TiS2 and compared it with the state of the art ARPES measurement. We have found that our band unfolding calculations give excellent agreement with the experiments, exhibiting the usefulness and validity of the band unfolding method. We have also applied the method to twisted-bilayer graphene.

From density functional to many-body Green's function and beyond

Wednesday 21 June 2017 09:30
Presenter: Prof. SUGINO, Osamu (The University of Tokyo)

Density functional theory has been sophisticated considerably by improving the functional form for the exchange, on-site Coulomb, and van der Waals interactions. After demonstrating an impressively successful application to the phase diagram of solid oxygen, we will discuss the problem of excited states and strongly correlated systems. For this purpose, we will review recent development of the first-principles many-body Green’s function method and, in addition, consider a possible future combination of nuclear physic and quantum chemistry.

Nuclear Gamow-Teller excitation and beta decay study within modern density functional theory

Wednesday 21 June 2017 11:15
Presenter: Dr. NIU, Yifei (ELI-NP)

The Gamow-Teller (GT) transition could be studied by charge-exchange reactions in the Lab, while it also happens spontaneously in nature, and is the dominant transition in □ -decay. □ -decay half-lives set the time scale of the rapid neutron capture process, and hence are important for understanding the origin of heavy elements in the universe.

I will introduce our recent study on GT transition and beta-decay with the quasiparticle random phase approximation (QRPA) + quasiparticle vibration coupling (QPVC) model. By including the QPVC effect, more correlations beyond mean field level have been introduced, therefore, the GT resonance spreading width, which cannot be described by the QRPA model, can be reproduced. The overestimation of beta-decay half-lives in the QRPA model are also solved by the inclusion of QPVC effect.

Development of two-component relativistic time-dependent density functional theory for Molecular Properties

Wednesday 21 June 2017 11:45
Presenter: Prof. KAMIYA, Muneaki (Gifu University)

In this work, we have developed the two-component relativistic time-dependent density functional theory with spin–orbit interactions to calculate linear response properties and excitation energies. The approach is implemented in the NTChem program. The two-component relativistic TDDFT with spin–orbit interactions was successfully applied to the calculation of the frequency-dependent polarizabilities and the excitation spectra of several molecules containing heavy atoms.

Quantized TDDFT dynamics

Thursday 22 June 2017 09:30
Presenter: Prof. NAKATSUKASA, Takashi (Center for Computational Sciences, University of Tsukuba)

In nuclear physics, the linearized TDDFT often fails to reproduce properties of low-energy modes of excitation. They are basically collective modes of a large amplitude nature, and the failure is due to missing correlations associated with these low-energy collective motions. The microscopic unified description of nuclear structure and reaction is also a big challenge for us.

In order to achieve these goals, we adopt a method to "quantize" the TDDFT on a selected collective subspace. In this presentation, I start from basic properties of nuclear system and basic idea of the methodology, then, show pedagogical model, and some recent pplications.

A quantum dynamics descriptor for exploring a mechanism of light-driven electron migration in molecular aggregated system

Thursday 22 June 2017 11:15
Presenter: Dr. YONEHARA, Takehiro (RIKEN)

We introduce a practical calculation scheme for the description of excited electron dynamics in molecular aggregated systems by using a locally group diabatic Fock representation. This scheme makes it easy to analyze the interacting time-dependent excitations of local sites in complex systems.

In addition, this scheme can treat light-matter couplings, spin-orbit and non-adiabatic couplings. The present scheme is intended for investigations on the migration dynamics of excited electrons in light-energy conversion systems associated with photo-chemical functionalities.

Quantifying the impact of plasmon and paramagnon effects in "conventional" superconductors from the first principles

Thursday 22 June 2017 11:45
Presenter: Dr. AKASHI, Ryosuke (University of Tokyo)

The advances in the density functional theory for superconductors in the recent decade have paved a way to non-empirical calculation of superconducting transition temperature (Tc) of real materials. The theoretical extensions are also under way to include the effect of electronic dynamical charge and spin fluctuaions with no adjustable theoretical parameter, which can be a first step toward a unified first-principles treatment of superconductors--from the conventional phonon to unconventional electron mechanisms.

With our recent first-principles results, we exemplify how and how much the dynamical charge fluctuation (plasmon) and spin fluctuation (paramagnon) effects modify the Tc in the typical phonon-mediated superconductors, which have previously been discussed in semiempirical manners.

Quantum phase transition and quantum self organization in nuclear to mesoscopic many-body systems

Thursday 22 June 2017 13:30
Presenter: Prof. OTSUKA, Takaharu (RIKEN/U. Tokyo)

Long-range exchange interactions in DFT and their significance in chemical reactions

Thursday 22 June 2017 15:15
Presenter: Prof. TSUNEDA, Takao (University of Yamanashi)

The significance of long-range exchange interactions is presented from the viewpoint of DFT in quantum chemistry [1] in the first part, and then, it is shown focusing on chemical reactions in the second part. So far, we have developed the long-range corrected (LC) DFT [2] and have applied it to a wide variety of chemical and physical properties [3]. As a result, we have confirmed that the long-range exchange interactions are required to calculate various types of the properties: e.g. charge transfer excitations [4], van der Waals bonds [5], nonlinear optical properties [1] and so forth. Orbital energies may be the most significant property that LC-DFT makes it possible to calculate quantitatively [6]. Since orbital energies are the solution of the Kohn-Sham equation, this indicates that the long-range correction essentially improves DFT (or exactly the generalized DFT). In the first part, I will briefly review our past studies on LC-DFT.

Recently, we are investigating chemical reactions using the quantitative orbital energies. As the exact orbital energies are proven to inhere, LC-DFT orbital energies hardly vary dependent on occupation numbers. Chemical reactions usually proceed through charge transfers in the initial processes. We found that LC-DFT orbital energies are kept almost constant in the initial processes of many reactions, and then, they rapidly increase toward the products [7]. We have recently developed an orbital energy-based reaction theory as the modification of conceptual DFT [8]. I will present this topic in the second part.

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Anderson-Bogoliubov phonon in inner crust of neutron stars

Thursday 22 June 2017 16:30
Presenter: Dr. INAKURA, Tsunenori (Niigata University)

Background: The Anderson-Bogoliubov (AB) phonon, called also the superfluid phonon, has attracted attentions since it may influence the thermal conductivity and other properties of inner crust of neutron stars. However, there are limited number of microscopic studies of the AB phonon where the presence of lattice nuclei is explicitly taken into account.

Purpose: We intend to clarify how the presence of lattice nuclei affects the AB phonon in order to obtain microscopic information relevant to the coupling between the AB phonon and the lattice phonon.

Methods: The Hartree-Fock-Bogoliubov model and the quasiparticle random-phase approximation formulated in a spherical Wigner-Seitz cell are adopted to describe neutron superfluidity and associated collective excitations. We perform systematic numerical calculations for dipole excitation by varying the neutron chemical potential and the number of protons in a cell.

Results: The model predicts systematic emergence of the dipole AB phonon mode, which however exhibits strong suppression of phonon amplitude inside the nucleus. We find also that the phonon amplitude around the nuclear

surface varies as the neutron density. At higher densities the AB phonon mode exhibits behaviour similar to the pygmy dipole resonance in neutron-rich nuclei.

Conclusions: The dipole AB phonon mode does not penetrate into the lattice nuclei. This suggests that the coupling between the AB phonon and the lattice phonon may be weak. It also may depend on the neutron density in a non-trivial way.

A unified description for strange quark matter objects

Thursday 22 June 2017 16:45
Presenter: Dr. XIA, Cheng-Jun (Ningbo Institute of Technology, Zhejiang University)

A unified description for strange quark matter (SQM) objects ranging from strangelets to strange stars is presented, i.e., the UDS model. The important differences on the properties of SQM objects resulted from introducing the UDS model and conventional treatments are discussed. The previously neglected effects such as charge screening, quark depletion, and electrons in conventional treatments are found to be important for the charge properties and stability of strangelets as well as the surface structures of strange stars, which are now well addressed in the UDS model.

Momentum-space quasiparticle RPA calculation with Skyrme energy density functional for rotating weakly-bound nuclei

Thursday 22 June 2017 17:00
Presenter: Prof. YAMAGAMI, Masayuki (University of Aizu)

We have constructed a new computer code for quasiparticle RPA (QRPA) calculation with Skyrme energy density functional. The matrix QRPA equation is diagonalized by the canonical basis of the Hartree-Fock-Bogoliubov states that break the spatial axial symmetry and the time-reversal symmetry. By using the Fourier-series expansion method, we can reduce the memory size and the computational time of calculations for rotating weakly-bound nuclei.

With this code, we discuss low-frequency quadrupole vibrations of weakly-bound nuclei around 40Mg. These nuclei have quadrupole deformation due to the broken magic number N=28. We emphasize that the coupling to the fluctuation of quadrupole pairing field generates the K=0 mode of quadrupole vibration. Eventually, this mode has strong sensitivity to the collective rotation. The microscopic structure will be clarified.

Cluster multipole theory for anomalous Hall effect in antiferromagnets

Thursday 22 June 2017 17:15
Presenter: Dr. SUZUKI, Michi-To (RIKEN-CEMS)

The modern formalism of the intrinsic anomalous Hall conductivity (AHC) provides profound insight into the AHE being closely related to the topology of one-electron energy bands [1,2]. Whereas the AHE is usually observed in ferromagnets and explained as an outcome of the macroscopic dipole magnetization, the AHE has been studied also for certain noncollinear AFM states by first-principles calculations [3,4]. Furthermore, a large AHC was recently discovered for the AFM states in Mn3Z (Z=Sn, Ge), whose magnetic geometry has no uniform magnetization [5-7].

We identified the antiferromagnetic (AFM) structures which induce the anomalous Hall effect (AHE) in spite of no net magnetization by introducing a novel concept, cluster multipole (CMP), to characterize macroscopic magnetization of antiferromagnets [8]. We applied the CMP theory to the noncollinear AFM states of Mn3Z (Z=Sn, Ge) and Mn3Ir and show that the AHE is associated with the cluster octupole moments which belong to the same symmetry as the magnetic dipole moments. We further compared the AHE in Mn3Z and bcc-Fe based on first-principles calculations and find out their similarity with respect to the CMP moments. The theory thus can also deal with the AHE in antiferromagnets on an equal footing with that of simple ferromagnets.

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From low-energy QCD to nuclear physics and energy density functionals

Friday 23 June 2017 09:30
Presenter: Prof. WEISE, Wolfram (TU Munich)

The interface of QCD at low energies with the physics of hadrons and nuclei is provided by an effective field theory of pions and nucleons based on the spontaneously broken chiral symmetry of QCD with (almost) massless u- and d-quarks. This presentation gives an overview of approaches to the nuclear many-body problem guided by these principles, using both perturbative methods and non-perturbative (functional renormalization group) strategies.

Applications to nuclear and neutron matter will be reported, with emphasis on stringent constraints at high densities implied by the existence of massive (two-solar-mass) neutron stars. The construction of an energy density functional will be described in this context and comparisons will be made with nuclear phenomenology.

Computational materials database toward discovering novel semiconductors

Friday 23 June 2017 11:15
Presenter: Dr. KUMAGAI, Yu (Tokyo Institute of Technology)

I would like to talk about our recently developing computational materials database, which is directed toward discovering novel semiconductors. I first illustrate why we need to build new database with existing databases developed by other groups. I then explain the technical issues and how to overcome them. Finally, I present current status of our database.

Development of the fragment molecular orbital method combined with DFT and DFTB and applications to proteins

Friday 23 June 2017 11:45
Presenter: Dr. FEDOROV, Dmitri (AIST)

In the fragment molecular orbital method (FMO), a molecular system is divided into fragments, and they are calculated in the electrostatic embedding of the whole system. Most standard quantum-mechanical methods can be used with FMO, including density functional theory (DFT), time-dependent DFT (TDDFT) and density-functional tight-binding (DFTB). The computational cost of FMO is nearly linear, enabling large scale molecular calculations. At the DFT level, that means hundreds or thousands of atoms, and at the DFTB level, a system composed of one million atoms was computed. The methodology of FMO will be briefly introduced and applications will be described, in particular, an application to proteins, which brings up the question of their HOMO-LUMO gap and metallicity of proteins as predicted by DFT and DFTB with some functionals. The role of long range corrections and solvent is very important for describing the electronic state of proteins.