Theoretical Studies on Novel Physical Properties Arising from Many-Body Interaction

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Education
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Professional Employment
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2011 Special Postdoctral Researcher, RIKEN
2013 Assistant Professor, The University of Tokyo
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2019 Associate Professor, Institute for Molecular Science
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Awards
2008 L'Oréal–UNESCO Japan National Fellowships for Women in Science
2011 Best Poster Award in ISSS-6 Internal Symposium on Surface Science
2017 Young Scientist Award of the Physical Society of Japan
2019 The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology
The Young Scientists' Prize
2020 The 1st Award for Early Career Women Scientists of the Japan Society of Vacuum and Surface Science
2021 The 2nd Fumiko Yonezawa Memorial Prize of the Physical Society of Japan

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Quantum many-body interaction is a source of novel physical properties in the condensed matters. In our group, we develop theoretical methods by combining quantum field theory and density functional theory, and carry out collaborative research with experimental groups. As specific targets, we focus on magnetism in nanostructure and energy dissipation.

For magnetism in nanostructure, we are interested in the Kondo effect and spin–orbit interaction. The Kondo effect arises from the interaction between the localized spin and conduction electrons, which forms a characteristic many-body state so called the Kondo singlet state. The spin–orbit interaction originating from relativistic effect constrains the direction of magnetic moment to specific direction. We investigate the possibility of novel physical phenomena induced by these interactions in the nanostructure and molecules on surfaces.

For energy dissipation, we focus on the effect of electron–phonon interaction. The electron–phonon interaction is one of the most fundamental interactions in the condensed matter physics, and the quantitative evaluation in realistic materials is highly demanding. We adopt the ab-initio calculation to analyze the signal of electron–phonon coupling in surface spectroscopy and thermal properties in various kind of solids.

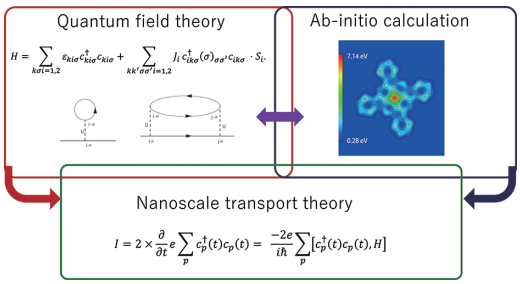

Figure 1. Schematic image of the theoretical method developed in our group.

Selected Publications

- E. Minamitani, N. Tsukahara, D. Matsunaka, Y. Kim, N. Takagi and M. Kawai, "Symmetry-Driven Novel Kondo Effect in a Molecule," *Phys. Rev. Lett.* **109**, 086602 (2012).
- E. Minamitani, R. Arafune, N. Tsukahara, Y. Ohda, S. Watanabe, M. Kawai, H. Ueba and N. Takagi, "Surface Phonon Excitation on Clean Metal Surfaces in Scanning Tunneling Microscopy," *Phys. Rev. B* **93**, 085411 (2016).
- E. Minamitani, N. Takagi and S. Watanabe, "Model Hamiltonian Approach to the Magnetic Anisotropy of Iron Phthalocyanine at Solid Surfaces," *Phys. Rev. B* **94**, 205402 (2016).
- R. Hiraoka, E. Minamitani, R. Arafune, N. Tsukahara, S. Watanabe, M. Kawai and N. Takagi, "Single-Molecule Quantum Dot as a Kondo Simulator," *Nat. Commun.* **8**, 16012 (2017).
- E. Minamitani, R. Arafune, T. Frederiksen, T. Suzuki, S. M. F. Shahed, T. Kobayashi, N. Endo, H. Fukidome, S. Watanabe and T. Komeda, "Atomic-Scale Characterization of the Interfacial Phonon in Graphene/SiC," *Phys. Rev. B* **96**, 155431 (2017).
- E. Minamitani, M. Ogura and S. Watanabe, "Simulating Lattice Thermal Conductivity in Semiconducting Materials Using High-Dimensional Neural Network Potential," *Appl. Phys. Express* **12**, 095001 (2019).

1. Ab Initio Investigation for Initial Process of Joule Heating in Semiconductor

Joule heating in semiconductors is a fundamental problem in solid-state physics. The resulting thermal damage, reduction in operational reliability, and power consumption of nanoscale transistors have become increasingly critical as the device size decreases. The macroscopic definition of the Joule heating is the dot product of the electric field and the current density. The microscopic process of Joule heating in a steady state is described as the energy balance between the electron and phonon intermediated by electron–electron, electron–impurity, electron–phonon, and phonon–phonon interactions under nonequilibrium conditions in the presence of a high electric field. Until recently, the empirical treatment of the band structure and the electron–phonon coupling prevents us from understanding the detail of relaxation process induced by these scattering process quantitatively and microscopically.

We propose a methodology for quantitative investigation of the energy relaxation process with the ab initio treatment of electronic states and electron–phonon interactions by approximating the nonequilibrium electron distribution function as being in equilibrium with an effective temperature.[1)] This approximation is known as the two-temperature model because the electrons and phonons are described by different effective temperatures, the electron temperature (T_e) and lattice temperature (T_l). The two-temperature model becomes reasonable if the electron equilibration time is sufficiently shorter than the time required for energy relaxation from electrons to phonons. Under such conditions, the Joule heating process can be described by the following three steps: First, electrons accelerated by an electric field are scattered elastically by electron–electron and electron–impurity interactions with a short relaxation time. This process randomizes the electron energy and momentum, and consequently, the electron distribution becomes isotropic in **k**-space, which can be described by a Fermi distribution with T_e. Second, the inelastic electron–phonon scattering with a longer energy relaxation time occurs, and the energy is transferred from the hot electrons to the cold phonons specified by T_l. Finally, the excited phonons are thermalized by the slow phonon–phonon interaction, and the heat energy is radiated to the environment or transported to a thermal bath such as a substrate and/or electrode by thermal phonons. We focus on the second energy transfer process as the initial step of Joule heating and develop a method to evaluate this process based on ab initio calculations.

Recent progress in ab initio calculations by combining density functional theory and the Wannier interpolation technique has enabled the evaluation of electron–phonon coupling with high precision. This technique has been employed to evaluate the transport properties of semiconducting materials. Here, we combine the ab initio calculation of the transport properties with the two-temperature concept. We applied this theoretical approach to bulk Si as a specific target.

As result, we found that the microscopic initial process of Joule heating differed in the electron and hole carriers. Figures 2 (a)–(d) show the phonon dispersion and decomposition of the energy relaxation rates into the contributions from the phonons with <27 meV, <50 meV, and >50 meV energy at low and high T_l as functions of E. The contributions from the phonons with medium energy, the LA and TO modes at the zone boundary, differ for the electron and hole carriers. For the electron carriers, there is a substantial contribution from medium-energy phonons at both low and high T_l. In particular, the relaxation via medium-energy phonons is dominant at low E at low T_l. In contrast, for the hole carriers, the contribution from medium-energy phonons is minor compared to that from the TO and zone center LO modes, except at a very low E at a low T_l. The origin of the differences can be attributed to the presence/absence of the intervalley scattering process and the isotropic/anisotropic band structures in the electron and hole carriers. The important factors that govern the energy relaxation process can be controlled by strain. A detailed ab initio investigation of the energy relaxation rate in a strained structure remains a topic for future research.

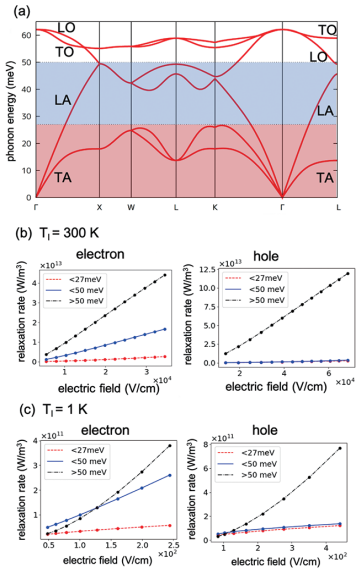

Figure 2. (a) Phonon band structure of bulk Si. The energy relaxation rates of electron and hole carriers are decomposed into contributions from phonons in the three energy ranges at (b) T_l = 300 K and (c) T_l = 1 K.

2. Other Ongoing Projects:
- Thermal Properties in Amorphous Solids

Reference

1) E. Minamitani, *Phys. Rev. B* **104**, 085202 (2021).

Awards

MINAMITANI, Emi; The 1st Award for Early Career Women Scientists of the Japan Society of Vacuum and Surface Science (2020).
MINAMITANI, Emi; The 2nd Fumiko Yonezawa Memorial Prize of the Physical Society of Japan (2021).
SHITADE, Atsuo; 15th Young Scientist Award of the Physical Society of Japan (2021).
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