Investigating R&D Committee on Applications of Quantum Chemical Computation in the Field of Electrical, Electronic and Insulating Material

Technical Committee on Dielectrics and Electrical Insulating Materials

1. Objective

Metals and semiconductor materials have periodic repeating arrangements of atoms in a crystalline structure. Theoretical analysis of their electronic structure is performed based on band theory, which has allowed for establishing a theoretical system connecting physical properties and electronic structures. On the other hand, band theory is not applicable to low-molecular materials such as gases and liquids, which do not have a regular structure. In addition to this, polymer materials, which have a complicated crystal structure owing to the existence of amorphous structures or chemical defects, hinder the theoretical understanding of the electronic structure of their dielectric and insulating properties. Recently, studies on these material peculiarities have commenced, seeking to analyze and understand the electronic structure of dielectric and insulating materials at the molecular level using quantum chemical calculation techniques. This has resulted in considerable research in Japan, which has produced consistent results. Therefore, this committee has been established to study domestic and foreign trends in the research of dielectric and insulating materials regarding quantum chemical calculation, discuss the results of the latest research, confirm the usefulness of quantum chemical calculations, secure the worldwide presence of Japanese research in these fields, and promote the use of quantum chemical calculations in the field of dielectric and insulating materials in Japan.

2. Background and internal and external research activities

Dielectric and insulating materials are a group of materials used in a wide range of fields to distribute electric energy in infrastructure and to ensure electrical insulation in various electric power equipment and home electric appliances. Gas, liquid, and solid phases are selectively used according to the application, with the addition of various innovations to promote the popularization of electric energy.

In recent years, it has become essential to expand and improve the functions and performance required of dielectric and insulating materials, as demand has increased to reduce environmental impact. This includes conversion to materials with low environmental impact, improving the efficiency of electric fields utilization in electrical equipment, responding to the active introduction of renewable energy, and responding to extreme conditions such as space and cryogenic environments. Although these material developments rely on performance verification based on experimental data, a more intrinsic understanding is considered necessary.

To address the challenges associated with such dielectric and insulating materials, research is being conducted to analyze the electronic structure of these materials using quantum chemical calculation and to discuss the relation between the electronic structure and physical properties. Several important findings are being reported by researchers in Japan.

The University of Tokyo, Tokyo City University, Kyushu Institute of Technology, and Shibaura Institute of Technology in Japan have reported findings based on quantum chemical calculation to derive physical property and their values. They are trying to estimate the macro electrical values of gases, liquids, and solids, and compare them with experimental measured values. In addition, a group at Kanto Gakuin University is attempting to analyze the generation and development mechanism of electric trees.

Overseas, ABB and others have constructed large-scale models simulating three-dimensional structures of crystalline and amorphous polymer materials and are evaluating the effects of additives and chemical defects based on quantum

chemical calculations. In addition, a few overseas organizations are trying to develop materials based on quantum chemical calculations under the Horizon2020 project, and the use of quantum chemical calculating technology is becoming a new trend in regional and national research themes.

3. Investigative matters

Research and investigation subjects based on quantum chemical calculation are listed below:

○ Current status of quantum chemical calculation

○ Examples of applying quantum chemical calculation to dielectric and insulating materials

○ Globally observed trends (regional and national)

○ Future potential of quantum chemical calculation

4. Expected effects

It is still too early to investigate quantum chemical calculation in the fields of dielectric and insulating material; a reliable understanding of quantum chemical calculation itself is first required. Then, by examining the latest research and ascertaining its aims and content, we shall identify the roles that quantum chemical calculation can play in dielectric and insulating material technology and disseminate that information to researchers and engineers. Thus, it is expected that there will be more researchers and engineers considering phenomena at the molecular level, which will open up new fields of dielectric and insulating material technology, as well as new approaches for gaining a fundamental understanding.

5. Term of investigation

December 2018 to November 2021

6. Committee members

Position	Name	Affiliation	Member/Non-member category of IEEJ
Chairperson	Satoshi Matsumoto	Shibaura Institute of Technology	Member
Member	Hiromitsu Asai	Denso Corporation	Member
〃	Daisuke Arai	Nagoya University	Member
〃	Takahiro Imai	Toshiba Infrastructure Systems & Solutions Corporation	Member
〃	Shinya Iwata	Osaka Research Institute of Industrial Science and Technology	Member
〃	Mitsumasa Iwamoto	Tokyo Institute of Technology	Member
〃	Hiroaki Uehara	Kanto Gakuin University	Member
〃	Takahiro Umemoto	Mitsubishi Electric Corporation	Member
〃	Naoya Kishi	Zeon Corporation	Member
〃	Akiko Kumada	The University of Tokyo	Member
〃	Muneaki Kurimoto	Nagoya University	Member
〃	Masahiro Kozako	Kyushu Institute of Technology	Member
〃	Masahiro Sato	The University of Tokyo	Member
〃	Ai Suzuki	Tohoku University	Non-member
〃	Yuji Suzuki	The University of Tokyo	Member
〃	Tatsuo Takada	Tokyo City University	Member
〃	Yasuhiro Tanaka	Tokyo City University	Member
〃	Kenji Toyota	Panasonic Corporation	Non-member
〃	Tomoki Hasegawa	Fuji Electric Co., Ltd.	Member
〃	Toshiyuki Hirano	The University of Tokyo	Non-member

Position	Name	Affiliation	Member/Non-member category of IEEJ
Member	Norikazu Fuse	Central Research Institute of Electric Power Industry	Member
〃	Masashi Yagi	Furukawa Electric Co., Ltd.	Member
Secretary	Yoitsu Sekiguchi	Sumitomo Electric Industries, Ltd.	Member
〃	Hiroaki Miyake	Tokyo City University	Member
Assistant secretary	Masamichi Kato	Yuka Industries. Co., Ltd.	Member

7. Activity schedule

Committee meetings: 2 times/year; Subcommittee: 2 times/year; Secretariat: 2 times/year

* The subcommittee is in charge of each field, and it is established for the purpose of investigating domestic and overseas research trends and reporting to this committee.

8. Reporting format

A technical report shall be prepared to present the results.