

ISAJ NEWSLETTER

An Initiative of ISAJ

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(we did not receive the article promised by the author, so maybe in the next issue...)


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<http://isaj.org>



Upcoming event: ISAJ organizes its 15th Annual Symposium on October 29, 2024!

Annual Symposium of ISAJ

ISAJ will organize its 15th Annual Symposium on October 29 (Tuesday) 2024 in Embassy's VCC Auditorium in Tokyo. This year's theme is "Transformative Technologies for a Sustainable Future." It will be organized by Dr. Sahiba Bano (NIMS Namiki), Dr. Deeksha Arya (U. Tokyo) and Dr. Aaditya Manjanath (NIMS Sengen).

Please submit your abstracts to make a presentation! Lend a hand in organizing; join the Organizing Committee!

ISAJ has been organizing an Annual Symposium since 2010. The primary objective of the symposium is to promote interaction and exchange of ideas among Indian and Japanese scientists. Over the years, the symposium has achieved many other objectives. Foremost is providing a platform to showcase the excellent science being done by Indian researchers and their colleagues in Japan to a wider audience.

Not the least important is the opportunity given to a large number of young Indian researchers in Japan to organize these symposia. Every year we have inducted motivated young researchers to convene the symposia by forming their own organizing committee. This endeavor works towards fulfilling our aim to bring up the leadership in our community of Indian researchers. We hope that they will lead our community in these changing times.

The symposia have been held in various locations, including the Embassy of India main auditorium, the University of Tokyo campus, the AIST auditorium in Tsukuba, Osaka University Hall, online, hybrid mode, Tokai University in Shizuoka, and Hokkaido University campus. With the rapidly increasing number of Indian researchers in Japan, it is now possible to organize symposia in each part of Japan (Northern, Tohoku, Kanto/Tokyo, Kansai, and Kyushu) every year.

15th ISAJ ANNUAL SYMPOSIUM
Transformative Technologies for a Sustainable Future
29th October 2024 (Tuesday)
Call for Abstracts
Submit abstract at convener@isaj.jp
Submission Deadline **10th Oct 2024**

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Information and Updates: www.isaj.org For more details, please refer the abstract template from [here](http://www.isaj.org)

**!!!Be an organizer of ISAJ events!!!
Join its executive committee!**

ISAJ is a non-profit organization that aims to elevate the profile and status of the Indian researcher and academic community in Japan. A number of volunteers have made it possible to organize the various activities of ISAJ, including its annual symposium, who have come forward due to their own motivation. It has been a lot of fun working together to organize truly multidisciplinary science events.

We call upon your initiative and dedication to organize ISAJ events in your area. You can submit your proposals and ideas to the Chairman of ISAJ (chairman@isaj.jp) for organizational support. We also invite you to join our organizing committee so that you can go ahead for implementing your ideas.

From Editor's Desk



Greetings and a warm welcome to the second issue of ISAJ Newsletter in 2024!

In this issue, we present you with one research article, an event report and a photo gallery, as well as about the upcoming 15th Annual Symposium.

The Research Spotlight is on “An atomistic deep dive into chemical reactions.” In this research, instead of an experimental chemical reaction, an unconventional computational route is applied to simulate reactions on supercomputers based on mathematical models. Using this approach, an understanding of the reactions is gained, which practically would be too fast to be observed experimentally.

The promised research highlight article did not arrive, so we may publish it in a future issue.

The event report is on the visit of the director of CSIR Advanced Materials and Processes Research Institute (AMPR), Bhopal, Dr. Avanish Kumar Srivastava, to National Research Institute for Materials Science in Tsukuba.

The photo gallery (back cover) is of a short symposium for visiting high school students which ISAJ organized in collaboration with Japan Education Center and Information (JECI) at the VCC auditorium of the Embassy of India in Tokyo.

ISAJ has reached a milestone in organizing its annual symposia. It is going to organize its 15th Annual Symposium this month on the 29th October. Its objectives and background is briefly given on inside cover.

We hope you would find the present issue of our Newsletter interesting. We look forward to receiving your feedback. Any suggestions/ideas for improving the upcoming newsletters are welcome.

Editor(s)
Alok Singh
Mahendra Kumar Pal

An atomistic deep dive into chemical reactions



Dr. Aaditya Majanath

Research Center for
Structural Materials,
National Institute for
Materials Science, 1-2-1
Sengen, Tsukuba, Japan
Email: man-
janath.aaditya@nims.go.jp

Aaditya is currently a NIMS Postdoctoral Researcher at NIMS, Tsukuba, Japan. He obtained his PhD from Indian Institute of Science in 2016 and has been involved in theory formulation and code development ever since. In his current position, he was instrumental in the development of a new methodology in the area of excited-state molecular dynamics known as time-dependent *GW* molecular dynamics (TDGW-MD) and has been employing it to study reactions pertinent to hydrogen production, human health, and radioactive water decontamination.

Introduction

A chemical reaction is a process which involves a transformation of one set of substances, known as the *reactants*, to another set, known as the *products*, either initiated by an energy input (*endothermic*) or followed by an energy release (*exothermic*). It is obvious that understanding chemical reactions helps us to fundamentally understand the world that we live in, better. Two types of approaches are available when investigating reactions – the conventional *experimental* route, wherein, the substances are actually combined together using a complex assembly of laboratory equipment in a planned manner, or the unconventional *computational* route, wherein, mathematical models based on fundamental principles of nature are used to simulate reactions on large computers (a.k.a. *supercomputers*). The computational approach may be the only viable option when trying to understand ultrafast chemical reactions that may occur at sub-picosecond (*pico* = 10^{-12}) timescales, which may either be difficult or practically unfeasible experimentally. The simulation tool that is used to study chemical reactions is *ab initio* molecular dy-

namics (AIMD), wherein, a feedback mechanism between the electronic and the nuclear degrees of freedom is embedded. The electronic/nuclear degrees of freedom involve solving the time-dependent (TD) Schrödinger equation (TDSE) for electrons/nuclei (shown for electrons in Figure 1 under “Electronic state”) to obtain the TD wavefunction (*wavefunction* – a mathematical function which is considered to contain the entire information of a system) of an electronic/nuclear state and the corresponding state energy. Typically, atoms are treated as classical particles as they are slower particles owing to their heavier masses compared to electrons. They are therefore, treated within the scope of Newton’s laws. An example schematic of the AIMD approach with the classical treatment of atomic motion is shown in Figure 1.

It is important to have an AIMD methodology that can accurately capture the atomistic intricacies of a chemical reaction. The current state-of-the-art, namely time-dependent density functional theory molecular dynamics (TDDFT-MD) has been used extensively used to study excited-state (ES) dynamics [1, 2], due to its ability to

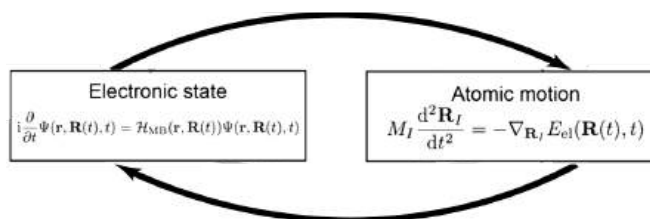


Fig. 1 Schematic of *ab initio* molecular dynamics where atoms are assumed to be classical particles and are treated through Newton’s laws.

handle large systems with a reasonable computational cost. However, it inevitably depends on adiabatic local density approximation (ALDA) [3], which is valid only for the initial state being the ground state and not for any initially excited state [4]. This is an important consideration when exploring the dynamics of endothermic processes such as photochemical reactions. The interested reader may be referred to our paper [5] for more information on the problems of TDDFT-MD with ALDA.

In response to the issues posed by the conventional dynamics methodology, we recently developed a novel method named non-adiabatic excited-state time-dependent *GW* molecular dynamics, or TD*GW*-MD in short [5]. Here, the accuracy of the *GW* method (which is known to fix the *band gap problem* to a great extent; *band gap problem* – the underestimation of band gaps in semiconducting/insulating materials via density functional theory, DFT, owing to technical problems in this method) is integrated into the dynamics framework to ensure that an accurate estimation of energies is in place, for capturing the chemical reaction dynamics correctly. We illustrate this via the example of the methane bond dissociation reaction $\text{CH}_4 \longrightarrow \text{CH}_3^\bullet + \text{H}^\bullet$ under photoexcitation (excitation of methane under light), in this article.

Workflow of TD*GW*-MD

Figure 2 shows a simple workflow of TD*GW*-MD. The first step involves reading (yellow-block in Figure 2) the structural information of the system, the electronic arrangement (or configuration) of the initial ES, etc. One prepares an ES by providing energy to the ground state. The ground state of a system can be considered to be the lowest energy state wherein, the electrons “prefer” to occupy certain energy levels as shown in Figure 3. By providing this external energy (in other words, *exciting* the system), an electron (blue-filled circles with arrows in Figure 3) can get pumped up from an occupied level to an unoccupied level, provided that the energy is sufficient enough. The next step in the workflow is to perform a DFT calculation (purple block in Figure 2) which essentially involves converging the electronic ES through a self-consistent procedure and obtaining the electron energies of the different levels. This is followed by correcting each of these energy levels through a *GW* step (sky-blue block in Figure 2). As

part of the dynamics procedure, we solve the TDSE for electrons using the accurate information obtained from *GW* and update the atomic coordinates for the next time instant using Newton’s laws (grey blocks in Figure 2). The entire looping process from the DFT step to the updating step continues till the number of MD steps defined by the user is reached.

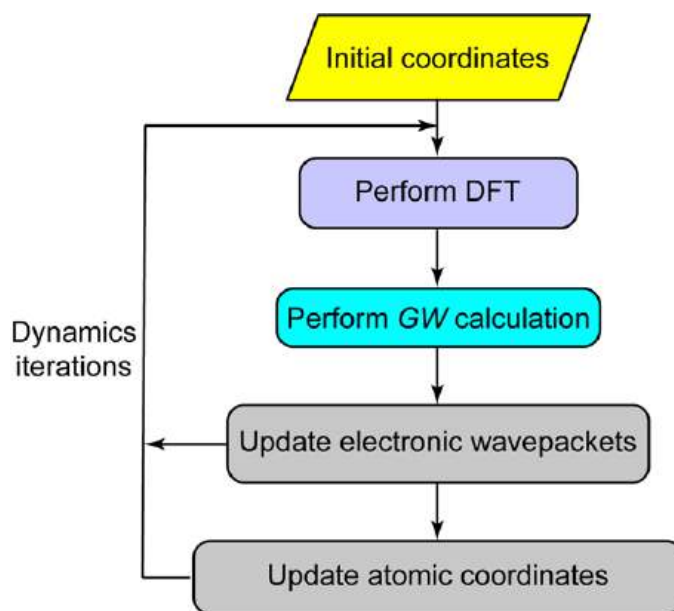


Fig. 2 A simple workflow of TD*GW*-MD.

Methane bond dissociation using TD*GW*-MD

We employ TD*GW*-MD to study the photolysis of methane, which is an important initiation reaction for hydrogen production towards alternative energy applications. The dynamics simulation starts with the excitation of an electron from the highest occupied molecular orbital (HOMO) to the lowest unoccupied molecular orbital (LUMO). This ES is shown in the right panel of Figure 3. Figure 4 shows the time-evolution of charge densities [panels (a)-(i)]. With progression in time, the excited electron is transferred from the methane fragment to one of the H atoms, which initiates the extension of the corresponding C–H bond and ultimately leads to a dissociation into the methyl CH_3^\bullet and H fragments about 34 femtoseconds (fs, *femto* = 10^{-15}) after the start of dynamics, showing that TD*GW*-MD correctly captures this dissociation dynamics. Table 1 provides further numerical evidence of the successful capture via TD*GW*-MD and also demonstrates why TD*GW*-MD is a superior method over TDDFT-MD.

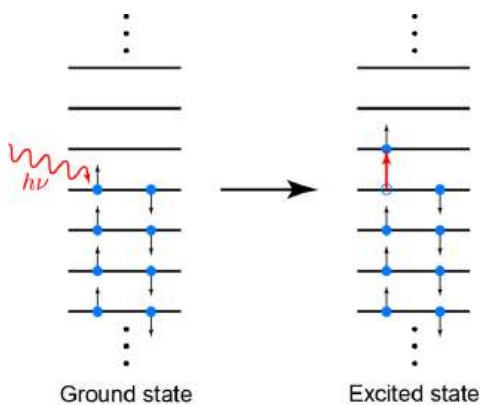


Fig. 3 A schematic of an excited state obtained through a photoexcitation of the ground state.

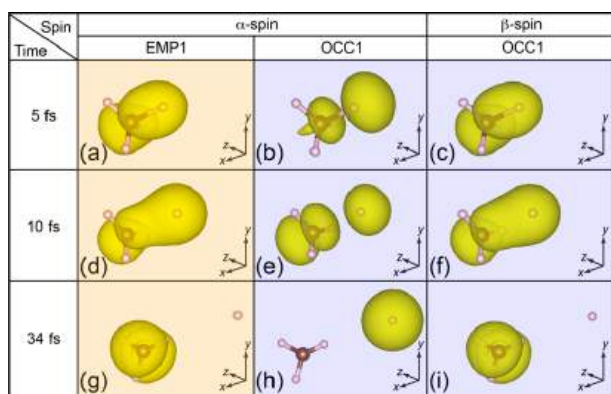


Fig. 4 Methane photolysis through TDGW-MD [5].

The values labeled by ‘a’ and ‘b’ refer to the experimental values of the different energy levels of CH_3^\bullet and H, respectively, while those labeled by ‘c’ are from TDDFT-MD simulations. The unlabeled values refer to the results obtained from TDGW-

MD. As is evident, TDDFT-MD severely underestimates the electron energies (by more than 4-6 eV, eV – electron-volts, a unit of energy at the atomistic scale) when they are compared with the experimentally reported values, due to the problems listed in Introduction. On the other hand, the TDGW-MD results are in very good agreement with those reported from experiments. For instance, the energy level OCC1 under the α -spin column in Table 1 corresponds to the H atom (charge density at $t = 34$ fs in Figure 4) and has a value of -13.2 eV from TDGW-MD which matches well with the experimental value for the isolated H atom, i.e., -13.6 eV (labeled by ‘b’ in the same column of Table 1). These observations indicate that TDGW-MD is a necessity when one intends to study ES chemical reactions accurately.

References

1. Y. Kodama and K. Ohno, *J. Chem. Phys.* **125**, 054501 (2006)
2. Y. Miyamoto and T. Komatsu, *Sci. Rep.* **9**, 12707 (2019)
3. M. Petersilka, U. J. Gossmann, and E. K. U. Gross, *Phys. Rev. Lett.* **76**, 1212–1215 (1996)
4. F. Cordova *et al.*, *J. Chem. Phys.* **127**, 164111 (2007)
5. **A. Manjanath** *et al.*, *J. Chem. Phys.* **160**, 184102 (2024)

Table 1 Comparison among TDGW-MD, TDDFT-MD, and experimentally reported results for the energy levels corresponding to the dissociated CH_3^\bullet and H fragments [5].

System	β -spin				α -spin	
	ϵ_{OCC4}	ϵ_{OCC3}	ϵ_{OCC2}	ϵ_{OCC1}	ϵ_{OCC2}	ϵ_{OCC1}
$\text{CH}_3^\bullet + \text{H}$	-23.7	-15.7	-14	-9	-13.5	-13.2
at $t = 34$ fs	-17.33^c	-11.55^c	-9.84^c	-5.46^c	-9.39^c	-7.61^c
CH_3^\bullet	-22.8	-16.3	-14.5	-9.8	-14.1	
geometry	-17.22^c	-11.45^c	-9.77^c	-5.38^c	-9.32^c	
at $t = 34$ fs					(HOMO)	
Planar CH_3^\bullet	-22.3	-15.1	-15.1	-9.7	-14.7	
	-16.81^c	-10.36^c	-10.36^c	-5.31^c	-9.92^c	
Planar CH_3^\bullet (experimental) ^a	-24.57	-15.64	-15.64	-9.84	-15.64	
Isolated H atom	-	-	-	-	-	-13.2
						-13.6^b
						-7.85^c
						(HOMO)

Visit of CSIR-AMPRI Director Dr. Avanish K. Srivastava

Renowned materials scientist Dr. Avanish Kumar Srivastava, Director of CSIR-Advanced Materials and Processes Research Institute (AMPRI), Bhopal, visited the National Institute for Materials Science (NIMS) at Tsukuba from July 4th to 5th, 2024. Dr. Srivastava was warmly greeted by Dr. Takahito Ohmura, Director of the Research Centre for Structural Materials (RCSM) at NIMS.



Dr. Srivastava presenting a steel idol of Lord Ganesha, 3D-printed fabricated at AMPRI.

Dr. Srivastava presented a talk entitled “New and Innovative Materials for a Range of Uses.” The talk was well attended by scientists, researchers and students engaged in diverse materials research. Dr. Srivastava presented recent research and technological breakthroughs from AMPRI in various domains, along with successful collaborations with industry and society. He also shared the CSIR-AMPRI success story in developing cutting-edge high-end indigenous Raman spectrometers.



Dr. Srivastava with DCM Mr. Madhu Sudan of Embassy of India, Dr. A. Singh of NIMS and Ms. Tansho of JSPS at the reception hosted by Dr. Panwar.

A research and scientific discussion session was organized for Indian postdoctoral researchers at NIMS. This session provided a platform for Indian researchers to discuss their work and explore collaborative and career opportunities with academic and R&D institutions in India. Dr. Srivastava discussed the ongoing projects, challenges and potential collaborative opportunities in AMPRI. The session was highly interactive. A personal interaction session was held in the evening at NIMS.

Dr. Srivastava also met several scientists/group leaders at NIMS to discuss possible future collaboration opportunities.

Dr. Srivastava was invited by Dr. Yashawant Dev Panwar, Counsellor (S&T), Embassy of India in Tokyo, to a reception on June 6, 2024, where Deputy Chief of Indian Mission Mr. Madhu Sudan, officials from Japan Society for Promotion of Science (JSPS) and several prominent scientists in Japan were present.



Dr. Srivastava with a section of audience after his talk at RCSM NIMS.



ISAJ organized a short symposium for visiting high school students in collaboration with Japan Education Center and Information (JECI)

Top: Speakers (left to right) Dr. Y. Ohmiya, Dr. A. Manjanath, Dr. A. Singh, Dr. R. Wadhwa, Dr. S. Kaul (ISAJ Chair), H.E. the Ambassador Mr. S. George, Capt. R. Adhikari (President JECI), Dr. Anubhav, Dr. R. Garg in the Embassy of India auditorium on 5 Aug. 2024.

Editors

Alok Singh, Ph.D.

National Inst. for Materials Science, Japan
quasi.sci@gmail.com

Mahendra Kumar Pal, Ph.D.

Indian Inst. of Technology (BHU), Varanasi, India
mail.mahendra.jpn@gmail.com

About ISAJ

The Indian Scientists' Association in Japan (ISAJ) is a Non-Profit Organization (NPO) aimed at networking and promoting Science and Technology Cooperation between India and Japan.

Contact Us:

Feel free to write to us

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