

Form B-2
(FY2022)
Must be typed

Date (日付)
20/09/2022 (Date/Month/Year: 日/月/年)

Activity Report -Science Dialogue Program-
(サイエンス・ダイアログ事業 実施報告書)

- Fellow's name (講師氏名): Gerardo Valadez Huerta (ID No. P20701)

- Name and title of the lecture assistant (講義補助者の職・氏名)

Non accompanying person

- Participating school (学校名): Suwa Seiryō High School

- Date (実施日時): 16/09/2022 (Date/Month/Year: 日/月/年)

- Lecture title (講義題目):

Molecular Simulation: Atoms meet computers

- Lecture format (講義形式):

◆ Onsite ・ Online (Please choose one.)(対面 ・ オンライン(どちらか選択ください。))

◆Lecture time (講義時間) 70 min (分), Q&A time (質疑応答時間) 20 min (分)

◆Lecture style (ex.: used projector, conducted experiments)

(講義方法 (例: プロジェクター使用による講義、実験・実習の有無など))

PowerPoint with real Molecular Models

- Lecture summary (講義概要): Please summarize your lecture within 200-500 words.

By imaging working as a chemist, the workplace might be a laboratory. Tools might be chemicals and instruments. The job might be to do experiments. It is not the whole truth. As a scientist, one can work everywhere in the world. Sometimes the tool of choice is a computer. (The fastest super-computer is made in Japan and is called Fugaku). The work might be the molecular simulation. Molecular simulation is based on quantum mechanics. In this lecture, the basics of Molecular Simulation were discussed by highlighting the contribution to this field of different renowned scientists. By solving the Schrödinger equation, one can predict all material properties. The Schrödinger equation can only be solved manually for the hydrogen atom. For other cases, computers are needed. The development of molecular simulation required a lot of theoretical work. Kenichi Fukui and his student Keiji Morokuma contributed significantly to the theory of chemical reactions. Sir John Anthony Pople and Walter Kohn developed computational methods to solve the Schrödinger equation. Further, the research at the Koyama Lab at Shinshu University by the JSPS Fellow is presented. This research concerns the investigation of new materials using

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molecular simulation. A Neural network atomic model is used. Finally, the importance of using English is summarized with real-life science examples

◆Other noteworthy information (その他特筆すべき事項):

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- Impressions and comments from the lecture assistant (講義補助者の方から、本事業に対する意見・感想等がありましたら、お願いいたします。):

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