

(For JSPS Fellow)

Form B-5

Date (日付)

20/09/2013

(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): Wessel Claudia (ID No. P12376)
- Participating school (学校名): Ishikawa Prefectural Nanao High School
- Date (実施日時): 18/09/2013 (Date/Month/Year: 日/月/年)
- Lecture title (講演題目): (in English) Introduction to Computational Chemistry
(in Japanese)
- Lecture summary (講演概要): Please summarize your lecture 200-500 words.

In my lecture I talked about my educational background and the motivation for becoming a researcher, my research topic and my home country Germany.

The theories of the research field *Computational Chemistry* were mostly developed during the beginning until the middle of the last century. Although they have been known for quite a long time, application of these theories to real problems was not possible until the end of the 20th century. This is due to the huge amount of computing power necessary for the calculations. But nowadays – as computers are becoming faster and cheaper – *Computational Chemistry* is becoming more and more popular.

Examples for the application of *Computational Chemistry*:

- Understanding of material characteristics which are not accessible by experimental means (for example complicated magnetic or electronic properties)
- Prediction of new compounds (of both already known and unknown types)

On the one hand *Computational Chemistry* is an aid to further understand already existing experimental data and on the other hand it helps the experimental chemist in finding new chemical substances by the theoretical prediction.

During the workshop I focused on the history of the atomic model and the impact *Quantum Physics* – the basis of *Computational Chemistry* – had on it. First I explained the models according to Rutherford and Bohr and then I talked about the nowadays picture of atomic orbitals. In the context of the modern atomic model I talked about the quantum numbers that determine the shape of an atom's orbital. For the interactive part of this workshop, the students worked in groups to figure out the electronic configurations of various atoms.

- Language used (使用言語): English with some Japanese words on the slides

- Lecture format (講演形式):

◆Lecture time (incl. workshop) (講演時間) 90 min (分), Q&A time (質疑応答時間) 20 min (分)

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

(講演方法 (例: プロジェクター使用による講演、実験・実習の有無など))

Projector

◆Interpretation (ex.: assistance by accompanying person, provided Japanese explanation by yourself) (通訳 (例: 同行者によるサポート、講師本人による日本語説明))

Assistance by accompanying person

◆Name and title of accompanied person (同行者 職・氏名)

1st year Master student Ogawa Yusuke

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

- Impressions and opinions from accompanied person (同行者の方から、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。):

今回このような高校生に科学の面白さを伝えるという立場になることになり通訳ながら、高校生が疑問に思う点が現在の自分とは異なっていたことに驚きを感じるとともに、高校生の物事のとらえ方が非常に興味深かったです。

また、英語での講義でさらに非常に高度なトピックであったのですが、積極的にわからないことを質問したり、我々が出題したクイズにも自分なりによく考えて解答していたことを通じて、テーマにとっても興味を示してくれていることが分かり、このような活動の意義がとてもあると感じました。