Must be typed

（For JSPS Fellow）

Form B-5

Date（日付）
（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）Krah, Alexander（ID No. P13705）

- Participating school（学校名）Aichi Prefectural High School Okazaki

- Date （実施日時）18.11.2013（Date/Month/Year:日/月/年）

- Lecture title（講演題目）:（in English） Research beyond borders − Research on ATP synthases
（in Japanese）

- Lecture summary（講演概要）: Please summary your lecture 200-500 words.

In my lecture I introduced Germany in its' nature and culture and I gave a short historical overview from the beginning of March revolution (first German democracy). I reported about daily life in Germany and pointed out some differences and similarities to the experiences I had in Japan. In addition I introduced the German higher education system and provided Pros and Cons for studying in Germany for foreign students.

In the second section, I talked about the daily life being a scientist. Thereofre I gave a short introduction how science is working and pointing out advantages and disadvanteges compared choosing a carreer in industries (from a German perspective due to the lack of knowledge of other countries).

In the third section, I introduce the work I have been doing since I arrived in Japan. Therefore I first introduce the method I am using (Molecular Dynamics simulations) and benefits applying this technique. I pointed out that this technique can help to interpret experimental data and propose new wet-lab experiments. Concerning the protein (ATP synthase), I am working on, I first introduced, how the protein works, followed by distinguishing between different mechanistic features in mammals and bacteria. I showed the students that MD simulations can be used to predict and explain experimental results and novel features features of proteins, based on the epsilon subunit of ATP synthases. Therefore I showed that we were able to predict a different ATP binding motif, as seen in the dimeric crystal structure, in the epsilon subunit of *thermophilic Bacillus* PS3, which does not apply to biology (monomer). In addition I showed that we can explain and predict a magnesium binding site in the epsilon subunit of *Bacillus subtilis*. This protein has been shown to bind magnesium, but aminoacids involved in the magnesium binding site have been unknown. With sequence comparison of the epsilon subunits from pathogenic bacteria, I proposed that the magnesium binding site might be present in some of these organisms. To show the students a structural basis, I presented homology models of the epsilon subunit from *Mycobacterium tuberculosis* and *Bacillus anthracis*, showing the before mentioned

magnesium binding motif. In addition I explained that experimental evaluation of the results, in connection with section 2 (collaborative environment in science), is beneficial and helps to varify results and extract reliable obtained from MD simulations. To show the students, that it might be important to understand the before mentined protein, I suggested some potential applications (biotechnological, drug design), which might be followed.

- Language used（使用言語）: English

- Lecture format（講演形式）:

◆Lecture time（講演時間）~90 min（分）, Q&A time（質疑応答時間）~30 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））
Use of projector.

◆Interpretation（ex.: assistance by accompanied 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））
No Japanese interpretation.

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

◆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。）: