受入大学名	大阪大学		
Host University	Osaka University		
外国人研究者	パダマ　アラン　アブラハム　ブストリア		
Foreign Researcher	Padama Allan Abraham Bustria		
受入研究者	ディニョ　ウィルソン　アジェリコ	職名	准教授
Research Advisor	Diño Wilson Agerico	Position	Associate Professor
受入学部/研究科	大学院工学研究科		
Faculty/Department	Graduate School of Engineering		

＜外国人研究者プロフィール/Profile＞

国　籍	フィリピン
Nationality	Filipino
所属機関	フィリピン大学ロスバニオス校
Affiliation	University of the Philippines Los Baños
現在の職名	准教授
Position	Associate Professor
研究期間	2019年8月3日　～2019年10月26日　（85日間）
Period of Stay	85 days (2019 / 08 / 03 - 2019 / 10 / 26)
専攻分野	計算材料科学・原子スケールモデリング
Major Field	Computational Materials Science / Atomic-scale Modeling

Padama, Allan Abraham Bustria

＜外国人研究者からの報告/Foreign Researcher Report＞

①研究課題　/　Theme of Research

Computational design of cheap and efficient hydrogen separation membranes

This study aims to computationally design potentially cheap substitutes to the expensive materials, usually precious metals, used in hydrogen separation membranes, for example when utilizing biomass, esp., agricultural wastes as hydrogen source. We study low cost transition metals considering their stability and performance towards hydrogen permeation.

②研究概要　/　Outline of Research

In this study, we determined the interactions of hydrogen atom (H) and hydrogen molecule (H2) with molybdenum (Mo) by performing density functional theory based calculations. We chose Mo because of its abundance in nature and of its bcc structure, which is favorable for H permeation. We determine the stable structure of bulk Mo, H and H2 adsorption, and the dissociation of H2 on the surface. In line with computational materials design, we also studied the optical properties of porous Si materials and the thermoelectric properties of half-Heusler alloys.

③研究成果　/　Results of Research

We found that the transfer of charge from the surface to the approaching H mainly characterizes the interaction of H with the surface. For the dissociation, the amount of energy needed to break the H-H bond strongly depends on the dissociation pathway of the molecule. The results suggest that a barrier-less or a facile dissociation of H2 is possible to happen on Mo(100) surface.
Below are the other activities during the period of my stay:
• Mentored graduate and undergradute students in the university;
• Gave lectures and short presentations;
• Attended academic workshops / lectures / seminars and workshop on scholarly publishing; and
• Discussed with collaborators and possible collaborators.

④今後の計画　/　Further Research Plan

We plan to do the following in the future:
• Investigate the effect of other molecules such as carbon monoxide on the adsorption and dissociation of H2.
• Examine H2 adsorption and dissociation, and co-adsorption with CO on Mo-(Transition Metal) alloy surfaces.
• Determine the behavior of ionized hydrogen on the surfaces.

＜受入研究者からの報告/Research Advisor Report＞

①研究課題 / Theme of Research

The researcher performed theoretical investigations on hydrogen–metal surface systems when he was a graduate student at Osaka University. His dissertation focused on the processes accompanying the interaction of hydrogen with metal surfaces. When he returned to his home country after his graduation in 2014, he continued to work on gas–surface systems. Motivated by current energy and environment issues, the gases he studied include carbon monoxide, carbon dioxide, and oxygen. The researcher has continued active collaborations with experimentalists in the Philippines and abroad.

②研究指導概要 / Outline of Research

The researcher performed investigation on Mo as a possible hydrogen membrane material, and also as a catalyst and as an electrode in nuclear fusion applications. In addition to doing research, the researcher has also be pro–actively involved in mentoring students of Osaka University, and continues to initiate discussions to explore and realize the establishment of new collaborations.

③研究指導成果 / Results of Research

The researcher was able to obtained vital results that would serve as benchmark in his future attempts to design more efficient materials for hydrogen related applications. The researcher was also involved in other collaborative researchers of the group, e.g., elucidation of the properties of porous materials for solar cells applications and effect of doping of alloys to improve their thermoelectric properties. With the pro–active involvement in these activities, the researcher should be able to extend his knowledge of materials design and benefit him in his future endeavors.

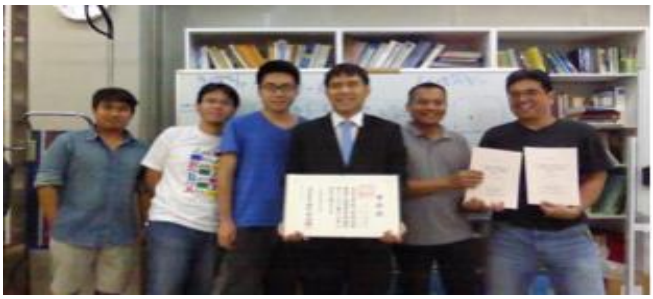
④留学生交流事業の活動状況 / Activities of International Student Exchange Program

The activities of the researcher during his stay include:
- Daily discussions and consultations with students.
- Regular meetings with Prof. Hideaki Kasai (President, National Institute of Technology, Akashi College)
- Weekly meetings with Prof. Yoshitada Morikawa (Department of Precision Science and Technology, Osaka University)
- Regular meetings with Prof. Nobuhiko Sarukura (Institute of Laser Engineering, Osaka University)
- Regular attendance in the Quantum Engineering Design Course workshops and academic seminars in Osaka University
- Attendance in the American Chemical Society workshop and discussions in publishing

⑤今後の計画 / Further Research Plan

The fellowship provided the researcher with opportunities to do research and at the same time experience the joys and challenges of being a leader, an educator, and a facilitator. These activities will continue in the future through joint research publications and projects, and exchange of students and researchers between our institutions.

Seminar at Applied Physics, Osaka University, August 30, 2019



Research Group Picture, Graduation Ceremony, September 25, 2019