

## Report for newly appointed faculty startup

1. Name of project leader : **Andrey Lyalin**

2. Project title: **Theoretical design of novel catalysts based on cheap and abundant elements.**

3. Report

In collaboration with Dr. K. Sakaushi (NIMS, Japan) we have described the current state of the art of experimental and theoretical investigations of quantum effects in proton transfer electrode processes [1]. Our work shed a light on the understanding of the fundamental mechanisms of key chemical reactions for the sustainable energy cycle, such as Oxygen Reduction and Hydrogen Evolution Reactions. Several domestic trips to NIMS, Tsukuba for scientific discussions and work with Dr. K. Sakaushi were very helpful for this research. In collaboration with the experimental group of Prof. Z. Huang (Univ. of Technology Sydney, Australia) we have developed a novel effective catalyst for the oxidative dehydrogenation of alkanes to olefins and demonstrated that the highly defective hexagonal boron nitride (h-BN) possesses outstanding performance for oxidative dehydrogenation of ethylbenzene to styrene [2]. We are planning to extend this research in the future and together with Dr. S. Kumar (Taketsugu group) investigate a wide variety of possible oxidative dehydrogenation reactions at the defective h-BN catalyst. The results of our research have been presented at several international meetings and helped to establish scientific collaboration with the experimental group of Prof. Dr. Knut Asmis (Leipzig Univ., Germany) with whom I am planning to start a new project on the investigation of the catalytic processes on size-selected metal oxide clusters. A novel single-phase structure of borophene (2D layer of boron) on Ir(111) surface has been discovered via a combination of computer simulations in ICRéDD and experiments in the groups of Dr. A. Preobrajenski (Lund University, Sweden) and Prof. Dr. A. Vinogradov (St Petersburg State Univ., Russia) [3]. This leads us to plan a new investigation of the physicochemical properties of novel stable borophene structures.

4. Research achievement

- [1] K. Sakaushi, A. Lyalin, and T. Taketsugu, Observations and Theories of Quantum Effects in Proton Transfer Electrode Processes, *Curr. Opin. Electrochem.* **19**, 96-105 (2020).
- [2] R. Han, J. Diao, S. Kumar, A. Lyalin, T. Taketsugu, Z. Huang, et al Boron nitride for enhanced oxidative dehydrogenation of ethylbenzene, accepted in *J. Energy Chem.* (2020).
- [3] N. A. Vinogradov, A. Lyalin, T. Taketsugu, A. S. Vinogradov, and A. Preobrajenski, Single-Phase Borophene on Ir(111): Formation, Structure and Decoupling from the Support, *ACS Nano* **13**, 14511-14518 (2019).