## The 85th GREEN Seminar



Theory-driven design of innovative catalytic materials for sustainable energy

Chair: Dr. Hidenori Noguchi (GREEN)

## Dr. Andrey Lyalin

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The problem of energy conversion and storage is an emerging issue for modern science. The lack of low-cost and efficient catalysts is the main factor limiting the use of sustainable energy technologies. Until recently the development of novel materials relied on experimental techniques, while theoretical methods were mostly used to rationalize experimental observations. However, with the increase in computer power and the development of novel computational methods theory becomes a very promising tool for materials design. In this talk, I will demonstrate how theory deeply integrated with experiments can lead to the development of novel catalytic materials. The main focus will be given to energy conversion processes, such as oxygen reduction reaction (ORR), oxygen evolution reaction (OER), hydrogen evolution reaction (HER), elementary processes in water electrolysis, and oxygen/hydrogen fuel cells.

Venue: Rm. 403, 4F, Collaborative Research Bldg.,

Namiki-site / Webex (Hybrid)

Date: Friday, March 3rd

Time: 11:00-12:00

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