

HU-ACE NEWS LETTER

Advanced Core for Energetics, Hiroshima University

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2021.1**Activities of the Core**

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| Jan. 8, 2021 | Prof. Aki's lecture was selected in Train Your Knowledge - Hiroshima University 100 Great Lectures. |
| Jan. 12, 2021 | The 91st Hiroshima University Biomass Evening Seminar (co-organized). |
| Jan. 14-29, 2021 | JICA Training Program "Biomass Utilization" |
| Jan. 15, 2021 | The 54th HU-ACE Steering Committee Meeting. |
| Jan. 27, 2021 | The 55th HU-ACE General Meeting |

HU-ACE cooperates in Carbon Recycling activities.

Since the declaration of "Japan's zero-emissions goal by 2050" was announced by Prime Minister Suga as part of his first speech in October 2020, carbon recycling technology has been attracting more and more attention. In addition, the president of Hiroshima University declared on January 26 that, "HU will achieve carbon neutrality by 2030". "Carbon recycling" is a technology that uses carbon dioxide as a resource and converts it into useful chemicals and fuels in order to reduce carbon dioxide in the air. This technology is indispensable to our research aims at HU-ACE. Many members of HU-ACE also cooperate with Hiroshima University's efforts related to carbon recycling research and development.

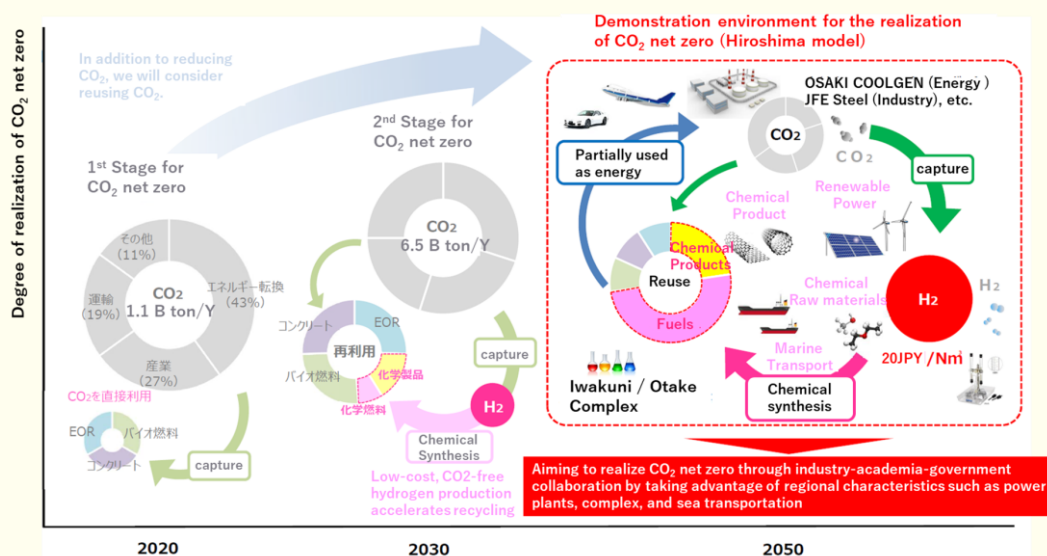


Figure The path to zero emissions of fossil fuels through carbon recycling



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Research fields: Computational chemistry, Computational material science, Energy engineering, Chemical system engineering

Keywords: Material MBR, Machine learning, Carbon-neutral, Hydrogen



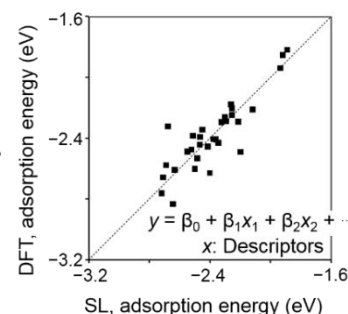
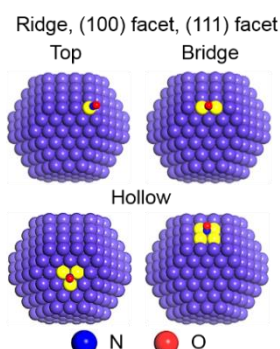
Abstract

Computational Chemistry & Material Informatics as Basis for Material Model-based Research

Activities at the Advanced Automotive Research Collaborative Laboratory started in October 2016, aiming at developing advanced materials for future automobiles. Especially, we are extending the concept of a model-based approach to material research, with our ultimate goal being controlling the mechanisms of automobiles at the electronic, atomistic and molecular levels.

Rare and precious metals are used in exhaust catalysis. Best utilizing the function of such rare elements is quite important to further realize high catalytic activity. Based on parallel computing using a supercomputer system, we were able to reveal NO (nitrogen monoxide) adsorption properties on Rh, Pt, Pd, Ag, Ir nanoparticles and predict the properties using machine learning [1].

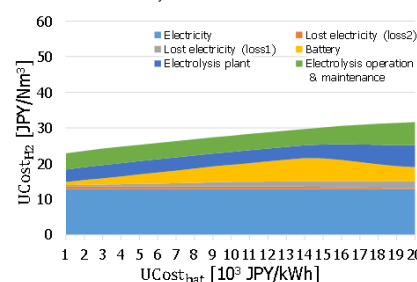
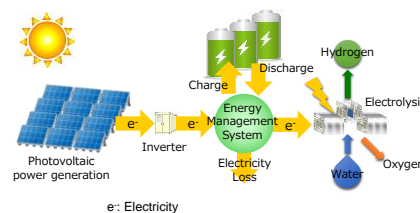
We are also collaborating with synthesis and measurement researchers on various material systems, aiming to create innovative materials.



Future System Design toward a Carbon-neutral Society

Toward a carbon-neutral society, massive utilization of renewable energy is inevitable. To best utilize variable renewable energy, energy storage is mandatory. Hydrogen is one of the candidates for long-term energy storage, however, its expensive production cost is well known.

We have applied an algorithm to search for an optimum solution from a vast parameter search space and have found that it is economically feasible by optimizing the system configuration [2]. It is noted that the system is effective in Japan, thus we expect to implement the system locally in Japan to best utilized local energy resources. To this end, we are collaborating with NPOs as well as finance companies.



References

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[2] Kikuchi, Y.; Ichikawa, T.; Sugiyama, M.; Koyama, M.: Battery-assisted low-cost hydrogen production from solar energy: Rational target setting for future technology systems, *International Journal of Hydrogen Energy*, **44**, 1451 (2019).