KOREA INSTITUTE OF ENERGY RESEARCH

**CP 7**

# CONCEPT PAPER

## for KIER International Cooperation project

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| **Title** | Development of the optimal composition & structure of heterogeneous catalysts based on the computational approach and atomic-scale characterization techniques | | | |
| **Description** | • **Barrier(s) to tackle:** Various heterogeneous catalysts have been developed to improve the performance and durability of energy devices and chemical processes. However, the catalyst development process has been inefficient since catalysts are mainly developed by experimental trial and error, which is costly and time-consuming. In addition, the compositions and structures of developed catalysts are often not fully optimized. We must substantially accelerate the development process of fully optimized catalysts guided by computational modeling and atomic scale characterizations in order to quickly commercialize direct methane coupling (DMC), hydrogen fuel cells, and renewable hydrogen production by $CH_4$ reforming.<br><br>• **Strategy to solve:** Periodic density functional theory (DFT) coupled with microkinetic modeling and machine learning (artificial neural network) will be used to obtain fundamental relationships between catalyst compositions, structures, and performance. Based on these relationships, we will identify the optimum compositions and structures of metal or metal-carbon hybrid catalysts for applications in the energy devices and chemical processes mentioned above. The theoretically identified optimum catalysts will then be synthesized, tested, and characterized based on atomic scale analysis such as AC-TEM, STEM, and EELS. By investigating the activation and deactivation mechanisms, we will also work on improving the durability of the fully optimized catalysts. | | | |
| **Outcomes*** | **Through the collaboration with KIER, the following outcomes will be obtained:**<br>• At least 2 hybrid catalyst models for the suggested energy devices (DMC, PEMFC, $CH_4$ reforming, etc.)<br>• Atomic scale characterization results of hybrid catalysts with mechanistic study<br>• Publications and/or Patents: 3 publications in SCI journals and 1 patent | | | |