iCeMS Kitagawa Group Seminar

Date: June 14th, 2019

Time: 16:30-18:00

Place: 2F Seminar room, iCeMS main building

Prof. Michihisa Koyama

Global Research Center for Environment and Energy Based on Nanomaterials Science,

National Institute for Materials Science (NIMS), Tsukuba, Japan

"Practical Applications of Computational Chemistry to Functional Material Systems and Its Perspectives in the Era of Data-driven Society."

ABSTRACT: Computational chemistry can play a key role in understanding functionality at the atomistic level, when it is appropriately applied to practical issues. Required computational approach will be different depending on the key for the functionality of the target: i.e. bulk/surface, interface, and higher order microstructure. First, I would like to introduce the application examples of first-principles study on the stability and functionality in various research disciplines, large-scale chemical reaction dynamics studied by using structure models reconstructed from HAADF-STEM observation, and a multi-scale, multi-physics simulations in the fuel cell and battery. Next, I would introduce an example of physics-centered AI integration; an approach to boost physics-centered researches by utilizing AI. Finally, future perspectives will be discussed.

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