RCMS Research Center for Materials Science, Nagoya University

Nagoya University

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Platform: Nano-Energy

Theoretical Chemistry Colloquium

February 9, 2015 (Mon), 16:00-17:00

RCMS, 2nd floor, Chemistry Gallery

Equivalence Class Sampling for Molecular Self-Assembly on Surfaces

Prof. Dr. Daniel M. Packwood
WPI-Advanced Institute for Materials Research (WPI-AIMR), Tohoku University

Abstract: An outstanding problem for materials chemistry is to predict a priori what kinds of structures are formed by self-assembly of molecules on metal surfaces. This presentation will introduce a mathematical model for exploring the thermodynamic stability of molecular assemblies on periodic surfaces. This 'block assembly model' is meant to capture some key aspects of bottom-up fabrication of graphene nanoribbons from organic precursors on copper surfaces (Han et al. ACS Nano 8, 2014, 9171).

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