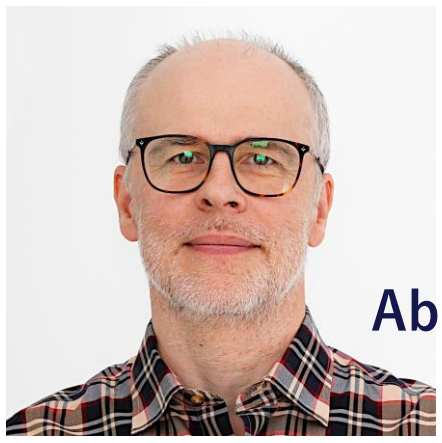
ICReDD International Seminar Series

Prof. Rafał Podeszwa (University of Silesia in Katowice, Poland)

CarbonGraphNET: Graph neural networks enter carbon chemistry

Place: Hokkaido University, CRIS building
ICReDD Salon (room02-106)



Time: Thursday, 10 December, 2026
15:00-16:30

Abstract.

Graph neural networks (GNNs) offer a unique opportunity to model systems based on their pure topology, enabling skipping of the expensive geometry optimization steps. For most chemical systems, where geometrical information is not uniquely determined by connectivity, such an approach would not work. However, for rigid carbon systems, GNNs allow efficient exploration of their vast isomeric space, owing to their high speed when executed on graphics processing units (GPUs). We present a GNN-based model that enables the complete exploration of larger fullerenes, containing billions of isomers.

A seminar organized by the
Taketsugu Group
(WPI-ICReDD, Hokkaido University)

Ambitious program for smart materials science, Hokkaido University