

“Materials research by Information Integration” Initiative (MI²I) Workshop

日時: 2017 年 7 月 27 日 13:30 – 17:40

場所: 千現地区第 2 会議室

13:30 – 13:45

Opening Address

Satoshi Itoh (NIMS)

13:45 – 14:45

Accelerating Materials Discovery with Data-Driven Atomistic Computational Tools

Chris Wolverton (Northwestern University)

14:45 – 15:30

Informatics-Aided Computational Design of Nanostructures for Thermal Transport

Junichiro Shiomi (The University of Tokyo)

15:30 – 16:00

Break

16:00 – 16:45

Materials Discovery by Combination of First Principles Calculations and Data-Centric Approaches

Isao Tanaka (Kyoto University)

16:45 – 17:30

Brute-Force First-Principles Sampling Investigations of Battery Electrolytes and Interfaces

Yoshitaka Tateyama (NIMS)

17:30 – 17:40

Closing remarks

Kiyoyuki Terakura (NIMS)