

**第3回極限物質科学研究会**  
**The 3rd Workshop for Extreme Materials Science**  
**“Structure and Properties of Silicate Glass/Melt”**

Date: 13:00-, Oct. 5th (Wed), 2016.

Place: Small Meeting Room 1(west), Welfare and Conference Bldg. (C61), Riken, Wako.

理研和光 統合支援施設小会議室 1 (西) 建物番号 C61

[http://www.riken.jp/en/access/wako-map/#campus\\_map](http://www.riken.jp/en/access/wako-map/#campus_map)

Organizer: Toshiaki Iitaka ( [tiitaka@riken.jp](mailto:tiitaka@riken.jp) )

Participation: Free

Sponsor: **Post-K Computer Challenging Problems, “Challenge of Basic Science”**,

Subproject C “Structure and Properties of Materials in deep Earth and Planets”

ポスト「京」萌芽的課題「基礎科学の挑戦」

サブ課題 C 「地球惑星深部物質の構造と物性」

<http://www.iitaka.org/~xmat/>

Co-Sponsor: Interdisciplinary Theoretical Science Research Group (iTHES),

理論科学連携研究推進グループ (iTHES)

[http://www.riken.jp/en/research/labs/rg/inter\\_theor\\_sci/](http://www.riken.jp/en/research/labs/rg/inter_theor_sci/)

Scope

Basics and applications of computational study of silicate glass/melt are presented: Dr. Noritake introduces his recent achievement on the theoretical study of sodium silicate liquid under pressure. Dr. Nguyen talks about calcium silicate under high pressure and its application to nuclear waste processing. Dr. Suzuki reports on the development of a molecular dynamics method using CONQUEST, a linear-scaling DFT code, for simulating silicate melts.

Program

13:00-13:10 **Toshiaki Iitaka**: Opening

13:10-13:40 **Fumiya Noritake**:

Ionic Liquid/Network Liquid Transition in Sodium Silicate Liquid: Molecular Dynamics Study

<http://fnoritake.futene.net/>

14:00-14:30 **Nguyen Van Hong**:

Structure of Calcium-silicate glass under high pressure

<https://sites.google.com/site/nguyenvanhongdnhbk/nguyenvanhong>

14:50-15:20 **Teppey Suzuki**:

大規模分子動力学シミュレーション手法の開発 (in Japanese)

Development of a Large-Scale Ab Initio Molecular Dynamics Method using CONQUEST

[http://www.nims.go.jp/cmsc/fps1/cmsu\\_fps\\_member.html](http://www.nims.go.jp/cmsc/fps1/cmsu_fps_member.html)

15:40 **Nguyen Van Hong**: Closing