

**第2回極限物質科学研究会**  
**The 2nd Workshop for Extreme Materials Science**  
**“Structure Prediction and Superconductivity”**

Date: Aug. 15th (Mon) 13:00-

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 ( [iitaka@riken.jp](mailto:iitaka@riken.jp) )

Participation: Free

Sponsor: **Post-K Computer Challenging Problems,**

Subproject “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/)

Program

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

13:10-13:40 **Maho Nakata**: The PubChemQC project: three million molecules data from quantum chemical calculations

<http://scitation.aip.org/content/aip/proceeding/aipcp/10.1063/1.4938866>

13:40-14:20 **Yanming Ma**: Pressurized hydrogen-rich compounds enroute to room temperature superconductivity

<http://www.calypso.cn>

<http://mym.calypso.cn>

14:20-15:00 **John Tse**: Superconductivity of high pressure hydride.

<http://physics.usask.ca/~tsej/>

(coffee break)

15:20-16:00 **Ryotaro Arita**: First-principles study on high T<sub>c</sub> superconductivity in sulfur hydrides

[http://fpmrt.riken.jp/public\\_html/index\\_en.html](http://fpmrt.riken.jp/public_html/index_en.html)

16:00-16:40 **Ryosuke Akashi**: Possible `Magneli` phases in sulfur hydride under high pressure

[http://a--k--c.com/index\\_en.html](http://a--k--c.com/index_en.html)

16:40-17:10 **Luciano Ortenzi**: Tight-binding model for cubic H<sub>3</sub>S: electronic structure and electron-phonon coupling.

<http://www.sapienza.isc.cnr.it/your-details/userprofile/mandrache.html>

17:10 **Ryotaro Arita**: Closing