

2020/04/12 [version 2.6/3.0]



# How to setup MaterApps LIVE!

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MaterApps LIVE! Development Team



# What are included in USB Stick?

- MateriApps LIVE! USB 
  - setup.pdf, setup-en.pdf  
this document
  - README.html, README-en.html  
(copy from <https://github.com/cmsi/MateriAppsLive/wiki/MateriAppsLive-ova>)
  - VirtualBox Installer: VirtualBox-\*-OSX.dmg, VirtualBox-\*-Win.exe  
(available at <https://www.virtualbox.org/wiki/Downloads>)
  - VirtualBox configuration scripts: vbconfig.\*  
(available at <https://github.com/cmsi/MateriAppsLive/tree/master/ova>)
  - MateriApps LIVE! VirtualBox Disk Image: MateriAppsLive-\*-amd64.ova  
(available at <http://sourceforge.net/projects/materiappslive/files/>)



# MateriApps — a Portal Site for Materials Science Simulation

- Aiming at the community formation through the promotion of application



since May 2013

- Introducing **271 materials science applications and tools** (as of 2020.4)
- Finding applications
  - search tags: features, targets, calculation methods/algorithms
- Information of applications
  - brief introduction, link to official pages, information installation, usage, etc
- Information of hands-on sessions, software update, etc
- Glossary of keywords, Concierge, Reviews
- 16000+ page views / month, 5500+ unique visitors / month

# Applications on MateriApps

- Introducing **271 materials science applications and tools**

## DFT

AkaiKKR★

OpenMX★

xTAPP★

ABINIT★

...

(78)

## Quantum Chemistry

FMO★

SMASH★

GAMESS★

DC★ ... (36)

## Molecular Dynamics

MODYLAS★

Gromacs★

ERmod★

MDACP... (31)

## Lattice Models

ALPS★

DSQSS

BLOCK

DMRG++ (52)

## Continuum Simulation

ANSYS Multiphysics

Octa ... (12)

## Data Analysis

CLUPAN★

phonopy★ (57)

## Visualization

fu★

TAPIOCA★ (37)

Database (11), Integrated Environment (4)  
Machine Learning (17), Quantum Computing (6)

★ included in MateriApps LIVE!



# Current status in computational materials science

- From developers' viewpoint
  - New algorithms should be implemented and used. Or, it will be forgotten ever existed.
  - It cost much to write and update documents
  - Development of software itself is hardly considered as scientific achievements
- From users' viewpoint
  - What kind of applications? Who develop them? Which application should I use for my problem?
  - Manual and documentation are not well prepared.
  - How to evaluate the accuracy of results?
- Goal of MateriApps project
  - **Forming of community in the field of computational materials science through the promotion of open source software**



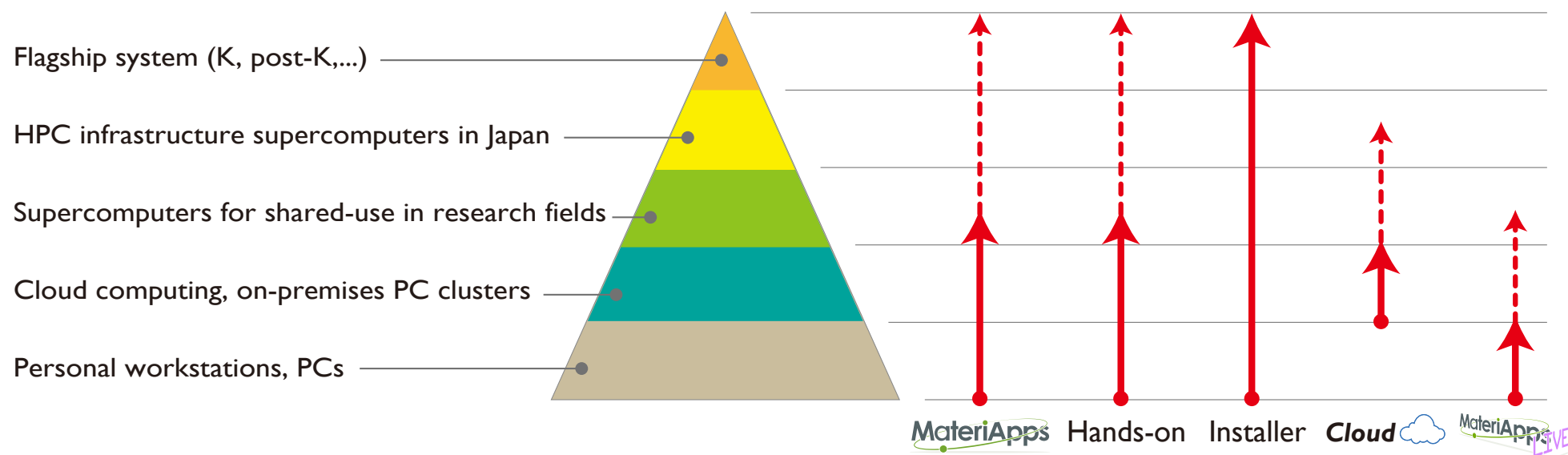
開発者



利用者

# What MateriApps will provide

- To find and learn application software
  - catalog of application/tool on **MateriApps web**
- To start using application software
  - **MateriApps LIVE!**
- To active use application software
  - pre-installation to the K computer, supercomputers, etc: **MateriApps Installer**

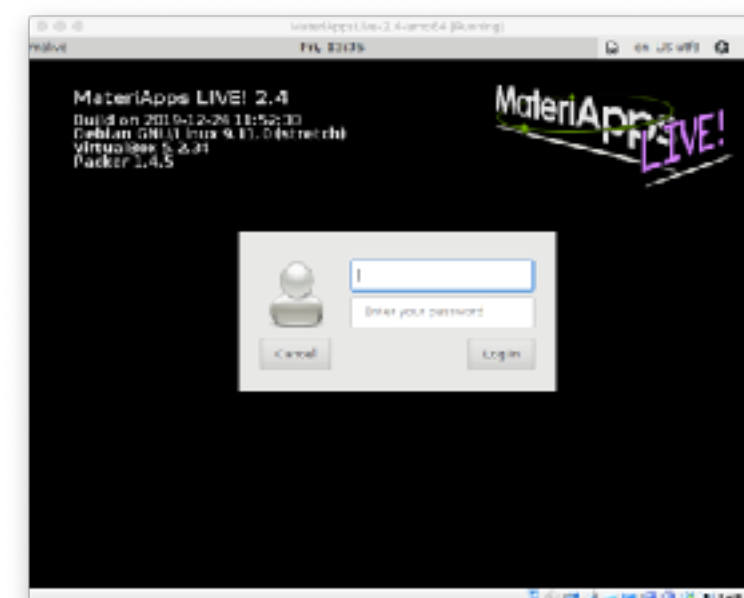
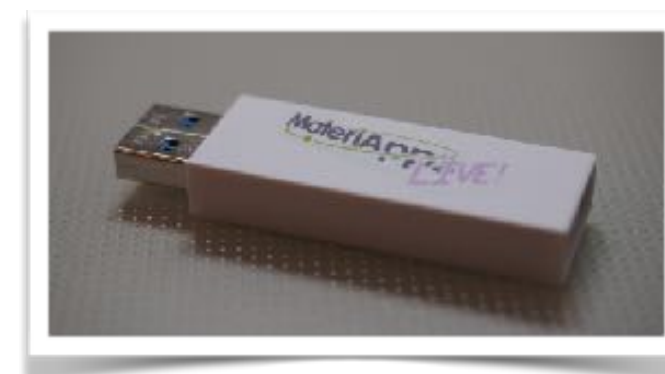


- Infrastructure for easily starting materials science simulations for theoreticians, experimentalists, researchers in companies, students, and more...

# What is MateriApps LIVE! ?



- Live Linux bootable on virtual machine
  - run on Windows, Macintosh, etc
  - just boot and get ready for materials science simulations without installation
- Version 2.6/3.0 was published in April 2020
- Pre-installed applications and tools
  - abinit, AkaiKKR, ALAMODE, ALPS, COQUEST, CP2K, DCore, DSQSS, H $\Phi$ , LAMMPS, mVMC, OpenMX, Quantum ESPRESSO, SMASH, xTAPP, etc
  - OVITO, ParaView, Tapioca, VESTA, VMD, XCrysDen...
  - GUI installer for CASINO, GAMESS, and VMD
- Available from MateriApps LIVE! webpage
  - c.a. 6600 copies distributed since July, 2013





# MateriApps LIVE! is useful for ...

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- Hands-on sessions using MateriApps LIVE!
  - MateriApps LIVE! Tutorials
  - $H\Phi$ , xTAPP, ALPS, DCore, mVMC, ALAMODE, DDMRG, DSQSS, SALMON, CASINO, etc.
- Practices in lectures
  - Computational Physics
  - Computer Experiments (UNIX + C, LaTeX, VCS)
- Used by experimentalists, researchers in private companies
- Used by researchers in the field of computer science
- Easy setup (c.a. 15min) without no troubles
- Useful for operation check, trouble shooting, user support

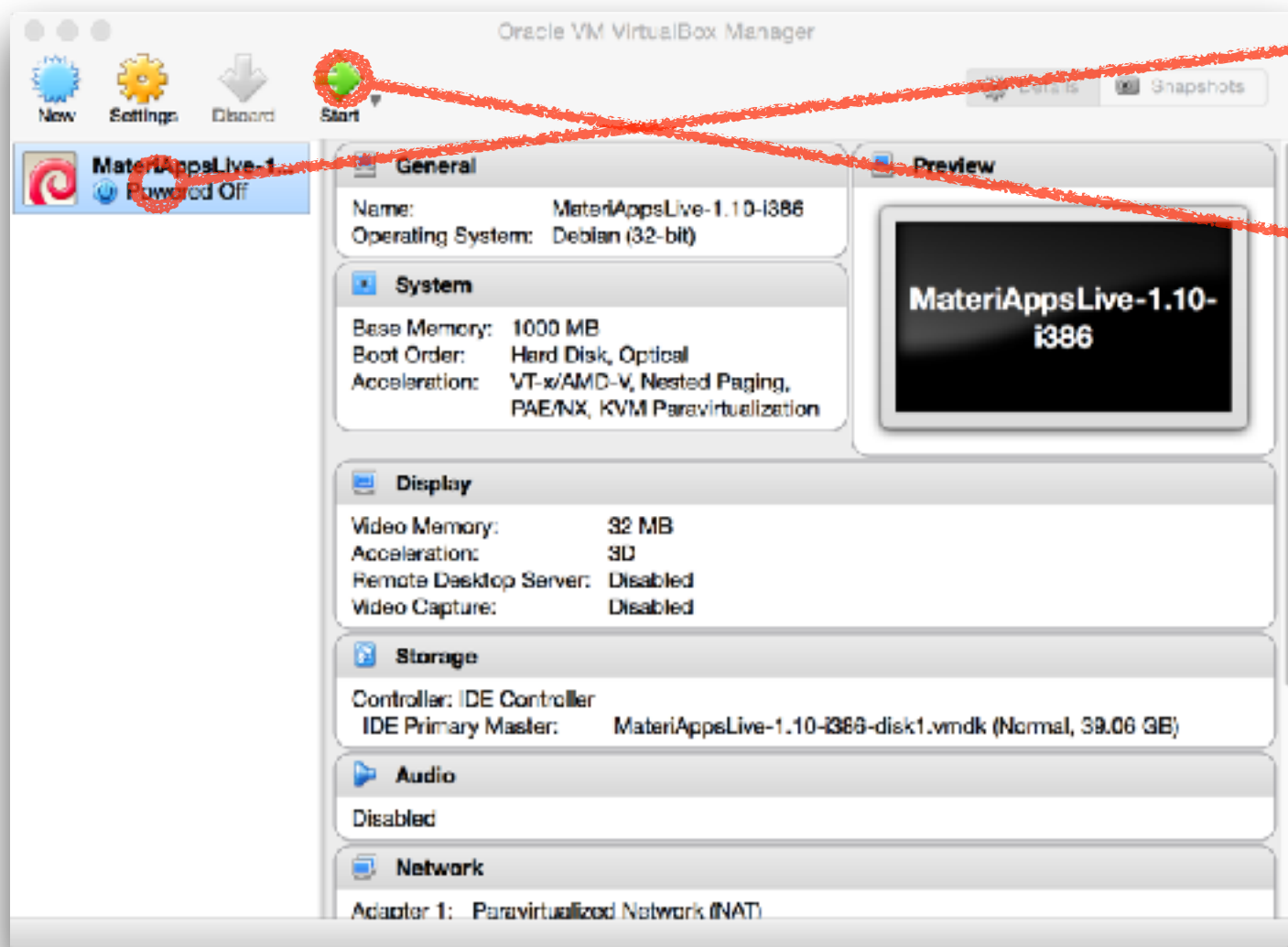


# Booting in VirtualBox

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- ✓ Copy files in USB stick memory to hard disk
  - copy all the files to your PC, e.g. to desktop
- ✓ Install VirtualBox by double-clicking the installer
  - For Windows: VirtualBox-6.\*-Win.exe
  - For Macintosh: VirtualBox-6.\*-OSX.dmg
- ✓ Import MateriApps LIVE!
  - double-click MateriAppsLive-\*.amd64.ova
  - VirtualBox will start automatically and import window will open. Then press “import” button
  - VirtualBox Manager window will appear in two or three minutes
- Host (host OS): operating system (Windows, Mac OS X, etc) on which VirtualBox is running
- Virtual machine (guest OS): operating system (= MateriApps LIVE!) running on VirtualBox

# Booting in VirtualBox

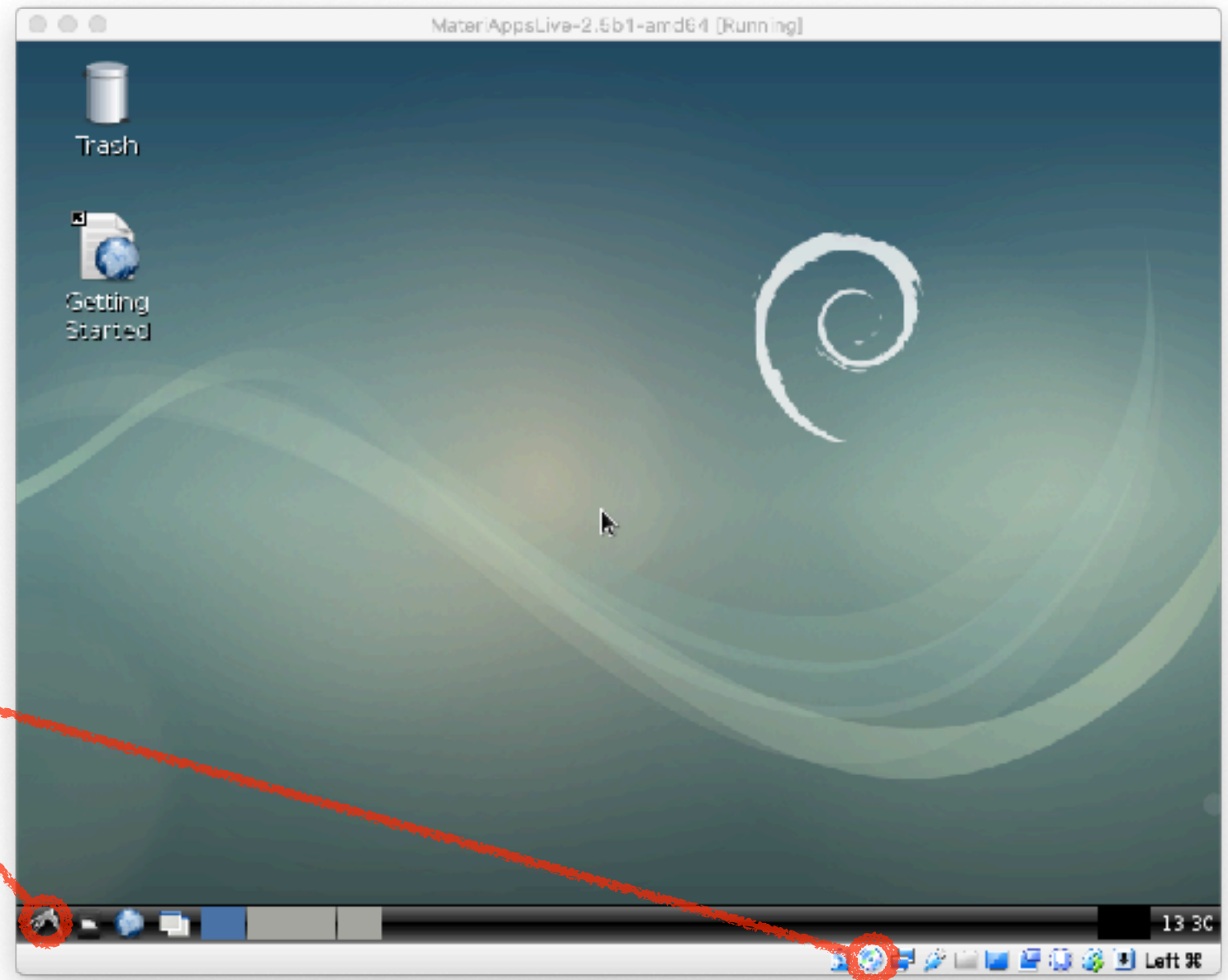


1. Choose "MateriAppsLive..."
2. Press "Start" button.
3. Wait until login window will appear.



# Login to MateriApps LIVE!

- Login window will appear in a few minutes
- Login by using
  - User name (login): *user*
  - Password: *live*
- Desktop (right) will appear
- Important buttons
  - *start menu*
  - *CD-ROM button*



# Tips (1/2)

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- ✓ Copy & Paste: How to paste strings copied from a PDF file on host OS?
  - right click on terminal window ⇒ “Paste”
  - or press “V” with “shift” and “control” keys
  - right click ⇒ “Copy”, or “shift + control + C” to copy a string
- ✓ Setting: using Japanese keyboard
  - start menu ⇒ “System Tools” ⇒ “Switch to Japanese Keyboard Layout”  
(or execute “*setxkbmap -layout jp*” in terminal window)
  - check if “@” key works correctly
- ✓ Setting: disabling unnecessary popup messages
  - on Windows: double click “vbconfig.bat”
  - on Mac OS X: double click “vbconfig.command”,  
or run “*sh vbconfig.command*” in terminal software



## Tips (2/2)

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- ✓ Settings: characters in the window are too small
  - “View” menu on the host OS, then choose “200%” in “Virtual Screen 1”
- ✓ Settings: browsing contents of ISO image file (\* .iso) from the virtual machine
  - click CD-ROM icon at the bottom of the virtual machine window frame, select “Choose disk image ...”, and select the ISO image file
  - contents of ISO image file are accessible via /media/cdrom0
- ✓ Setting: file sharing between host OS and virtual machine
  - choose MateriAppsLive-\* in VirtualBox Manager window, then “Settings”
  - open “Shared Folders” tab and click “+” on the right
  - click “v” on the right of “Folder Path”, choose “Other...”, and select the folder to which the files have been copied from the USB stick memory
  - check “Auto-mount” box and press “OK”. Then press “OK” again
  - the folder specified above can be accessed as /media/sf\_... after rebooting the virtual machine

# Materials Science Simulation by MateriApps LIVE!

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- Introduction / Setup
- First-principles band calculation (OpenMX / Quantum ESPRESSO / xTAPP)
- Simulation of solution by molecular dynamics (LAMMPS / Gromacs)
- Lattice model simulation (ALPS / H $\Phi$  / mVMC)
- Quantum chemistry calculation (in preparation)
- Hands-on materials are available at <https://github.com/cmsi/MateriAppsLive/wiki/MaLiveTutorial> (currently only in Japanese)



# MateriApps planning & production

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- Administration:
  - Center for Computational Materials Science, Institute for Solid State Physics, University of Tokyo (ISSP-CCMS)
- MateriApps Development Team
  - Kota Ido (ISSP), Shusuke Kasamatsu (Dept. of Phys., Yamagata Univ.), Takeo Kato (ISSP), Naoki Kawashima (ISSP), Hikaru Kouta (ISSP), Takahiro Misawa (ISSP), Yuichi Motoyama (ISSP), Syngye Todo (Dept. of Phys., Univ. of Tokyo/ISSP), and Kanako Yoshizawa (RIST)
- Cooperation:
  - Research Organization for Information Science and Technology (RIST)
  - Materials research by Information Integration Initiative, NIMS (MI2I)
- Sponsor
  - Post-K Priority Issue 7
  - Elements Strategy Initiative
  - Professional Development Consortium for Computational Materials Science (PCoMS)
  - TIA “Kakehashi”