Electronic Materials Center: TIES **Director：Hideo Hosono (Tokyo Tech)**

Creation of novel materials & devices with universal issues clarified

Project Outline for the 2nd Phase（FY2016–2018）

- Further evolution in the challenging exploration of new materials with expanded target materials based on novel concepts, structures & compositions
- Concentration on candidate materials for industrialization
- Starting collaborative research with industry partners in the four areas of focus shown in the figure to the right

Semiconductors
- Areas lacking in Japan's mainstream
- High-mobility, bipolar, ultra-wide bandgap
- Novel doping methods
- P-type amorphous semiconductors
- Nitrides, Sulfides、Hydrides
- Dirac electron systems

High-k dielectrics/ferroelectrics
- For power electronics at high T
- Stable oxygen deficiencies
- Abundant & nontoxic elements
- Non/low-dimensional perovskytes
- Non-oxide nitrides/oxynitrides
- Hydrides

Roles & Functionalities of Hydrogen
- Heretofore ignored existance and roles of hydrogen in oxides
- Quantification & state analyses
- Correlations between hydrogen and electronic states
- Hydrogen as a functional element
- Novel hydride materials

Collaboration of theory & synthesis

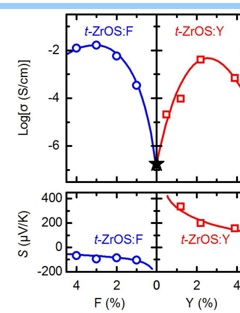
Rapid screening
- Calculation methods taking defect states into account
- Theoretical prediction of synthesis routes
- Materials informatics

Research Results (FY2016–2018)

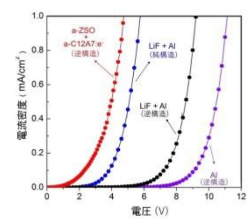
◆Novel Semiconductors & Devices

1. ZrOS: bipolar semiconductors based on early transition metals
2. Zn-Si-O (ZSO): high-performance nanostructured semiconductors composed of abundant elements for electron transport in OLED
3. Cu-Sn-I: p-type amorphous semiconductors with the highest mobility

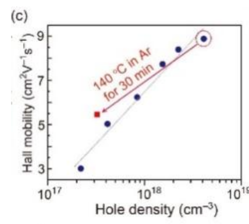
[1] T. Arai, *et al.*, *JACS* **139**, 17175-17180 (2017).
[2] N. Nakamura, *et al.*, *Adv. Electron. Mater.* **46**, 1700352 (2018).
[3] T. Jun, *et al.*, *Adv. Mater.* **30**, 1706573 (2017).



Bipolar transport of ZrOS



I-V characteristics of OLED with electron transport layer of Zn-Si-O

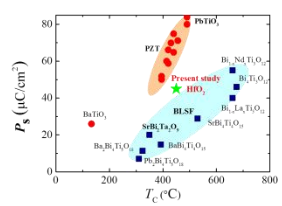


High Hall mobility (9 $cm^2V^{-1}s^{-1}$) of solution processed a-Cu-Sn-I

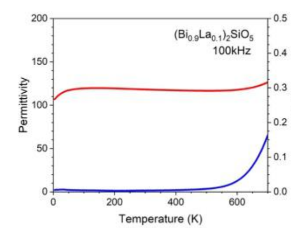
◆Non-Perovskite Dielectrics for Power Electronics

1. HfO_2:Y: fluorite ferroelectrics with high T_C & P_S
2. BSO ($(Bi_XLa_{1-X})_2SiO_5$) ：silicate dielectric with high ε_r at high temps satisfying standard requirements for automotive power electronics
3. CTAS ($Ca_3TaAl_3Si_2O_{14}$): Langasite piezoelectric for automobiles

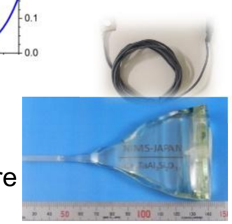
[1] T. Shimizu, *et al.*, *Sci. Reps.* **6**, 32931 (2016).
[2] H. Taniguchi, *et al.*, *Phys. Rev. Mater.* **2**, 045603 (2018).
[3] X. Fu, *et al.*, *Cryst. Growth. Des.* **16**, 2151-2156 (2016).



HfO_2:Y positioning in T_C-P_S correlation



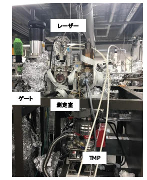
Constant temperature dependence of BSO


CTAS single crystal and prototype pressure sensor module

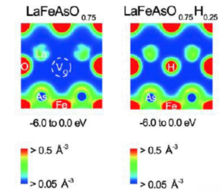
◆Quantification & State Analysis of Hydrogen (H)

1. Highly sensitive (10^{16} cm^{-3}) quantification of H in condensed matter
2. Discovery of hydrides in the amorphous oxide semiconductor a-IGZO and elucidation of their roles in the instabilities of transistor devices
3. Superior stability of hydrides to V_O in iron pnictide superconductors
4. Pressure dependence of superconducting H_XS by DFT calculations

[1] T. Hanna, *et al.*, *Rev. Sci. Instrum.* **88**, 053103 (2017).
[2] J. Bang, *et al.*, *Appl. Phys. Lett.* **110**, 232105 (2017).
[3] Y. Muraba, *et al.*, *Inorg. Chem.* **54**, 11567 (2015).
[4] R. Akashi, *et al.*, *Phys. Rev. Lett.* **117**, 075503 (2016).

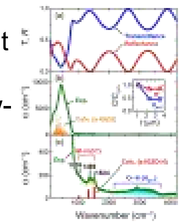


Discovery of hydrides by FTIR & DFT in a-IGZO

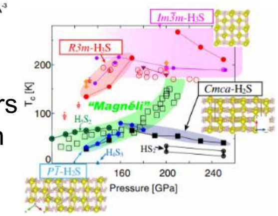


DFT elucidation of high T_C H_XS

Development of system to measure low-density hydrogens



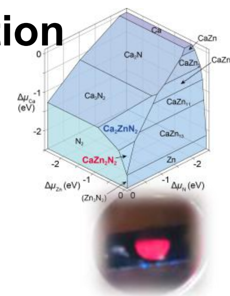
V_O in iron pnictide superconductors substituted with hydrides



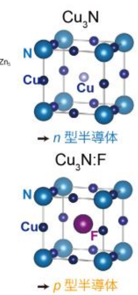
◆Typical Results of Theory-Synthesis Collaboration

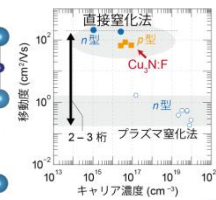
1. $CaZn_2N_2$: red-light emitting novel nitride semiconductor demonstrated by materials informatics and high-pressure synthesis
2. Ca_3N:F: DFT-based theoretical prediction and experimental demonstration of p-type doping of interstitial fluorine
3. Sr_5P_3: novel intermetallic 1D electride theoretically predicted by exploration based on GA and experimental demonstration

[1] Y. Hinuma, *et al.*, *Nat. Comms.* **7**, 11962 (2016).
[2] K. Matsuzaki, *et al.*, *Adv. Mater.* **30**, 1801968 (2018).
[3] J. Wang, *et al.*, *JACS* **139**, 15668 (2017).

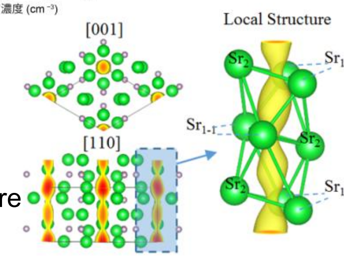


Theoretically predicted phase diagram and red-light emission from $CaZn_2N_2$





Interstitial fluorine doping for p-type Cu_3N

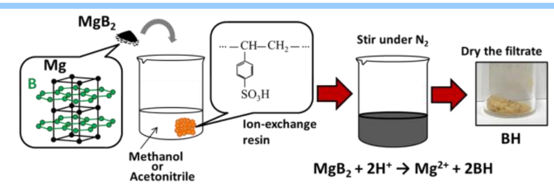


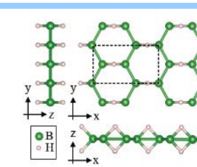
Crystalline and electronic structure of Sr_5P_3

◆Other Remarkable Achievements

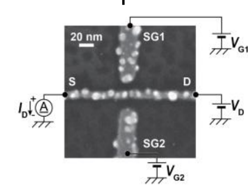
1. BH nano sheets: discovered novel covalent two-dimensional electronic materials
2. Single-molecule resonant-tunneling transistor: demonstrated a channel of a few nanometers and operations aiming at achieving high-speed electronics

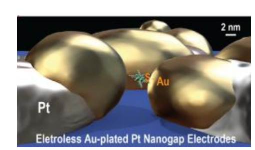
[1] H. Nishino, *et al.*, *JACS* **139**, 13761 (2017).
[2] Patent pending (2018).

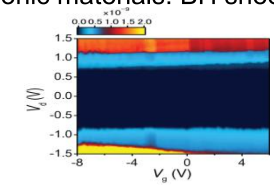




Fabrication process for two-dimensional electronic materials: BH sheets







Device structure and I-V characteristics of COPVn single-molecule resonant-tunneling transistor