Director: Hideo Hosono (Tokyo Tech)

Creation of novel materials & devices with universal issues clarified

Project Outline for the 3rd Phase (FY2018–2021)

- Transfer of technologies to industry: novel semiconductors for flat-panel displays and high-k dielectrics for power electronics
- Publication of records on the concepts, approaches, materials design methodologies, and achievements
- Evolution to post TIES (NEW Element Strategy)

in the four of the focused areas as shown in the right figure

Research Results (FY2019)

Novel Light Emitting Semiconductors & Devices

 Low-temperature and solution processed halide perovskite LEDs (PeLEDs) with ETL of a-Zn-Si-O (ZSO) emitted green light (525 nm) with high brightness (~5 × 10⁵ cd⋅m⁻²), power-efficiency (33 lm⋅W⁻¹), and narrow band (~15 nm)¹

Potential solution to green-gap issues of GaN-based LEDs



L/I-V of green PeLED with a-ZSO



¹ K. Sim, *et al.*, Appl. Phys. Rev. **6**, 031402 (2019, Featured). ² T. Jun, *et al.*, APL. Mater. **7**, 111113 (2019).



and electronic statesHydrogens as functional elements

Novel hydride materials





- Calculation methods with defects
- Theoretical prediction of synthesis routes
- Materials Informatics

\blacklozenge Database of V_{o} electronic states in oxides

- Comprehensive calculations based on automatic high-throughput methods developed by the end of 2nd phase of the project.
- Completely original database found nowhere else.
- Oxides having hydrogen-like Vo states can be understood from trends of transition states and explored with machine learning.¹
- ¹ F. Oba, et al., Ceramics Japan 54 (2019).

•Novel ternary nitride semiconductor with direct E_{a}

- Novel material of red-light emitting wurtzite CaZn₂N₂ was discovered by M.I. and high-pressure synthesis in the 2nd phase of the project.
- In FY2019, rock-salt MgSnN₂ and CaSnN₂ were predicted and synthesized by metathesis reaction under high pressure.¹
- To be applied to green light-emitting devices (E_{a} ~2.4 eV).
- ¹ F. Kawamura, et al., Euro. J. Inorg. Chem. 2020, 446 (2019).

Novel functional hydride (hydride conductor)

- TIES has focused on states, small quantity of hydrogen, exploration of functional hydrides in condensed matters.
- It is demonstrated that LaH_{3-2x}O_x shows extremely high conductivity of hydride ions (H⁻) ($2.6 \times 10^{-2} \text{ S} \cdot \text{cm}^{-1}$) by unharmonic oscillation¹
- Exploring chemical and electrical applications.
- ¹ K. Fukui, et al., Nat. Comms. 10, 2578 (2019).

Super high-speed electronics by single-molecule FETs

- Stable nano-gap (a few nm) electrodes were developed.
- The nano-gap was connected by a single molecule.
- Single electron FET and resonant tunneling FET were demonstrated by the single molecule FETs.
- To be applied to super high-speed electron devices.
- ¹ S. J. Lee, et al., Appl. Phys. Exp. **12**, 125007 (2019).



ion conductivity





Collection of band alignments

NaCl + 10 wt.% ZrO₂

$E_{\alpha}^{opt} = 2.4 \text{ eV}$ /arb. $hvF(R)]^2$ Birds-eye view 1.0 2.0 2.5 3.0 $MgF_{2}+SnF_{4}+6NaN_{2}$ Photon energy, hv / eV Cross section Optical absorption Metathesis reaction furnace

Direct

