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Development of next-generation quantum material research platform

Overview

- The present project aims an international collaboration, mainly between Japan and USA, for developing the next-generation quantum material research 'platform'.
- The platform contains several scalable quantum material simulators and data scientific analyzers.
- We will concentrate on developing software components that can be used commonly with simulators.
- The platform will be built on Oakforest-PACS.
- An international workshop is planned on 4. Dec. at U Tokyo.

Members

\[\text{Leader: Takeo Hoshi (Tottori U)}
\text{Deputy Leaders: Ashiro Nakano (U. South California)
Yasuaki Yamamoto (U Elect. Comm.)}
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Kohji Shimamura (Kobe U)
Shigemori Tanaka (Kobe U)
Fujiki Shimojo (Rikukawa U)
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Concept

The whole research activity, simulation and data science, are carried out on a supercomputer.

Large-scale quantum material simulator (1): ELSES

- Fig. 4: Research example: ELSES for poly-(phenylene-ethynylene) (PPE) (See the below figure).
- The foundation of ultra-flexible device or the next-generation Internet of Things (IoT) products, like display, lightening device, sensor and battery.
- The structural disorder in organic polymer is crucial for device performance or the mobility (Terasa et al. Nat. Commun. 4, 1699(2013)).
- Fig. Examples of organic material devices: (a) Sumitomo Chemical Co. (b) Sony (c) U. Tokyo. (d) Konika Minolta (e) Watanabe, et al., KONICA MINOLTA TECH. REP. 13, 16 (2016)

Organic polymer research as a combined research between large-scale simulation and data science (2)

- Strategy for data science:
  - The device performance (mobility) can be estimated by the quantum wave function by the k-means clustering method (not shown) or
  - Step 4. Solve the classification problem of the 40,000 samples
  - Prototyping the next-generation material research in large material

Organic polymer research as a combined research between large-scale simulation and data science (3)

- Procedures of data scientific analysis:
  - Step 1. Prepare 450,000 samples of disordered organic polymer with 1200 atoms on a GPU (See the below figure)
  - Step 2. Calculate the electronic states for each polymer by ELSES
  - Step 3. Calculate the participation ratio of electronic states, a measure for the spatial extentaion, for each wavefunction.
  - Step 4. Solve the classification problem of the 40,000 samples by the f-measure clustering method (not shown) or
  - Fig. Structure of disordered poly-(phenylene-ethynylene) (PPE) (See the next page).

Note: The organic polymer research of pp.6-9 was carried out in the collaboration with Koji Hukusima (U. Tokyo) and Hiroto Imachi (Tottori U). The current affiliation: Preferred Networks Inc.;
T. Hoshi et al., JPS meeting, Mar. (2017) and Sep. (2017); Paper in preparation.