Large-scale device-material research by massively parallel electronic structure calculation and data science

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The present project was carried out for the joint research between electronic structure calculations and data science. Related mathematical studies and software development were also carried out. The main collaborators are Yusaku Yamamoto (U. Elec. Comm.), Koji Hukushima (U. Tokyo), Takatoshi Fujita (IMS), Hiroyuki Matsui (Yamagata U.), Toshio Hyodo and Ayahiko Ichimiya (KEK).

The large-scale electronic-state and transport calculations were carried out for flexible organic devices. As a main achievement, principal component analysis (PCA) was carried out so as to analyze large-scale electronic state calculation data for exploration of organic polymer device materials [1-3]. The method is given by the dimensional reduction of electronic wavefunctions, since the original data size is huge. The reduction is realized, when the participation ratio of wavefunctions, a measure of quantum localization, is chosen as the descriptor. The computation was carried out for electronic states for 40,000 samples of disordered organic polymers with 1,200 atoms by our large-scale electronic state calculation code ELSES (http://www.elses.jp/) on the K computer. As results, the polymer samples are classified into four groups correctly and the physical meaning of the principal components is clarified. The present method is general and forms a rigorous foundation of the data-driven material science. Numerical methods for large-scale electronic state calculations were developed for efficient contour integral [4], intermediate eigenpair computation [5], middleware for parallel eigenvalue computation with the performance prediction function by Bayesian inference [6]. In addition, preliminary researchs were carried out for large-scale exiton calculation of organic interface [7] and large-scale electronic state calculation of disordered pentacene thin film [8], the development of data analysis on positron diffraction experiment [9].

As mathematical studies, we developed a new preconditioner for the CG method which combines the block red-black ordering with relaxed modified incomplete Cholesky factorization. Numerical experiments on a multicore processor shows that the preconditioner is both effective and scalable [10]. We also developed a new algorithm for the nonlinear eigenvalue problem based on signed singular values [11].

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