

A data scientific research on organic polymer device materials

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Preliminary results are reported of our data scientific research on organic polymer device materials with fast numerical computations. The purpose is a prescreening procedure of large-scale electronic-state simulations with quantum wavepacket dynamics, so as to explore a organic polymer with better device performance or higher mobility value [1]. Polymers are flexible (soft) and industrial polymers form fairly disordered structures. Various disordered structures should be considered and we should choose ‘hopeful’ structures before the quantum dynamics simulation. Here we picked out poly-(phenylene-ethynylene) (PPE), a typical organic polymer. The previous simulation research [1] implies that the non-uniform rotation angles among benzene rings, θ in the inset of Fig. 1, are crucial for the locality of the π electron wavefunctions and the device property.

As the first research stage, a classification analysis of the disordered polymer structures was carried out; (Step I) We prepared two-hundred structures with randomness. The structures were generated into two groups with small and large rotation angles. (Step II) A singleshot calculation was carried out for each structure so as to obtain the Hamiltonian and overlap matrices. (Step III) The generalized eigenvalue problem in each structure is solved numerically for the partial eigenpairs only for the π electrons. The method is based on the contour integral formula with several distinguished features. The features, including low or high accuracy control, multiple level parallelism, user selected wanted eigenvalue regions, allow us to solve the generalized eigenvalue problems efficiently. (Step IV) The participation ratio (PR), a measure for the spacial extension of wavefunction, is calculated for each wavefunctions (eigenvectors). Each structure is reduced to a list (vector) of the PR values. (Step V) The structures are analyzed, for the PR values by the k-means

clustering analysis, a famous data scientific method for the classification. The result is shown in Fig.1. The analysis works fine, since it classifies the structures into the two groups, as expected.

[1] T. Hoshi, talk in this workshop.

Fig. 1(right) The k-means clustering (classification) analysis for disordered polymer structures.

