Measurement and analysis of electrical conductivity of single molecular devices

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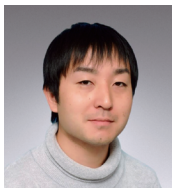
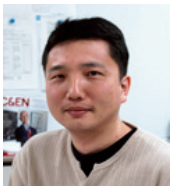




Abstract

Single-molecule devices attract attentions because of possible bottom-up construction, potential for device miniaturization, and utilization of unique electrical responses of organic materials. Since it is not possible to directly observe the bridging structure of the molecule between electrodes, the presence of the molecule should be confirmed through the current-voltage characteristics. We have developed a method to unveil the junction structures by combining the break junction technique, unsupervised clustering, and first-principles calculations and applied it for a tripodal anchoring molecule.

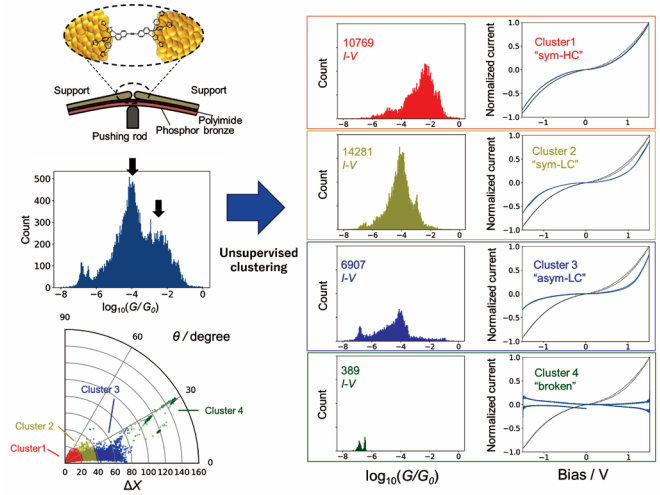
Background & Results

The research field “single molecule electronics” aims for realizing the smallest electrical devices fabricated by a bottom-up method. The break junction method, which is widely used to measure the electrical conductivity of single-molecule devices, is a method in which a narrow gold wire is slowly stretched and broken while measuring electrical conductivity. If a molecule is bridged between electrodes in a certain probability, the electrical conductivity of the molecule appears as a peak in the accumulated conductance histogram. This measurement is normally performed more than thousands of times, and the resulting histogram becomes broad. Such a broad distribution originates from the multiple junction structures, exhibiting different electrical conductivities depending on the bridging structures, while classification of the peaks is not feasible.

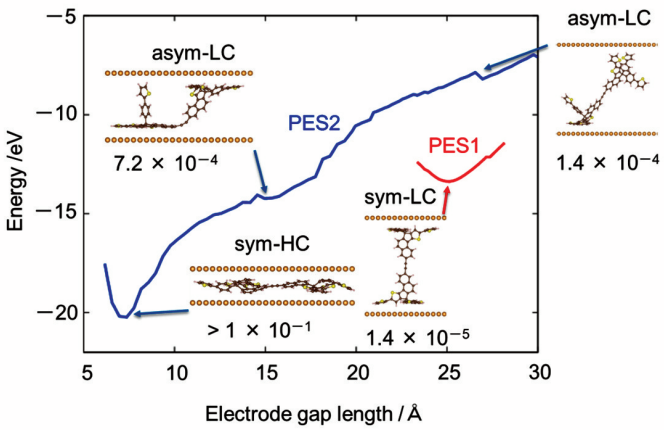
On the other hand, the measurement data of the break junction method is considered to be suitable for application of data science methods, because the data possesses so-called 3V (volume, velocity, and variety) characteristics of big data. In this study, we analyzed the break junction data of a tripodal anchoring molecule using unsupervised clustering. By employing the similarity between the averaged current-voltage curve and the individual current-voltage curve as the feature value, all the data could be classified into three electrical conductivity peaks. First-principles calculations also suggested that the existence of three different bridging structures characterized by the conductivity and contact asymmetry. This method will be useful for the analysis of single-molecule junctions with various bridging structures.

Significance of the research and Future perspective

By using unsupervised clustering, which is one of the data science methods, a large amount of data could be classified into meaningful clusters, which could be linked to the molecular bridging structures. In the future, we aim for more precise analysis by applying state-of-the art data science techniques and accurate theoretical predictions of structure-conductivity relationship using quantum computers.



Schematic diagram for the mechanically controllable break junction (MCBJ) measurement and the obtained conductance histogram. The arrows indicate the peak conductances. Clusters obtained by vector-based feature values in the k-means clustering method (k = 4) is also shown. The right panel shows the conductance histograms calculated from the I–V curves for clusters 1–4 and the normalized I–V curves averaged within each cluster and. The reference I–V curves, R, are represented by the black dotted lines.



Potential energy surfaces and conductance values calculated by density functional theory for the metastable molecular junction structures. We assumed two series of potential energy surfaces (PESs) and calculated the molecular binding energy by changing the electrode gap length. PES1 has a deep minimum, where the molecule achieves the self-standing structure. On the other PES (PES2), one of the tripodal anchors was laid on its side and there are several minima. These structures would appear during the formation of molecular junctions after the contact of two electrodes.

Patent

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Keyword single molecular electronics, break junction, first-principles calculation, machine learning