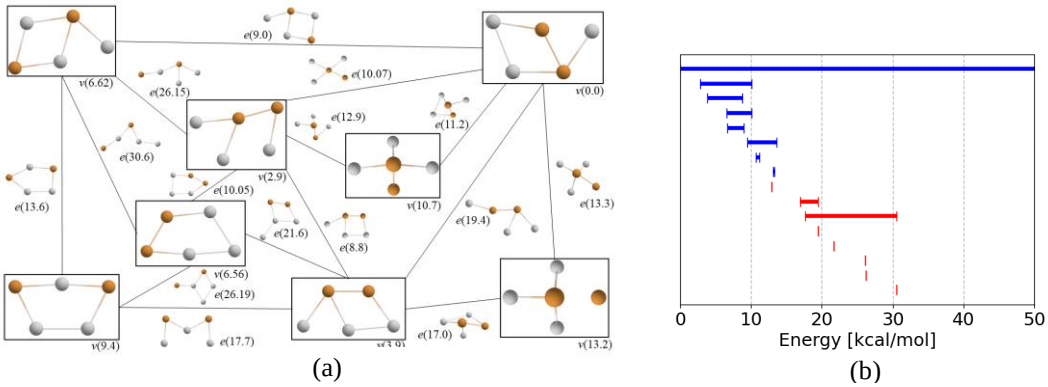
Characterizing Reaction Route Map of Realistic Molecular Reactions based on Weight Rank Clique Filtration of Persistent Homology

Burai Murayama[1], Masato Kobayashi[2,5], Masmitsu Aoki[2], Suguru Ishibashi[2], Takuya Saito[2], Takenobu Nakamura[3], Hiroshi Teramoto[4], and Tetsuya Taketsugu[2,5]

[1]*Graduate School of Chemical Sciences and Engineering, Hokkaido University, Kita 10 Nishi 8, Kita-ku, 060-0810 Sapporo, Japan*
[2]*Faculty of Science, Hokkaido University, Kita 10 Nishi 8, Kita-ku, 060-0810 Sapporo, Japan*
[3]*National Institute of Advanced Industrial Science and Technology, 1-1-1 Umezono, 305-8568 Tsukuba, Japan*
[4]*Faculty of Engineering Science, Kansai University, 3-3-35 Yamate-cho, 564-8680 Suita, Japan*
[5]*WPI-ICReDD, Hokkaido University, Kita 10 Nishi 8, Kita-ku, 060-0810 Sapporo, Japan*

In theoretical studies, chemical reactions are clarified by means of the potential energy surface (PES), which is a scalar function on $3N-6$ variables in the case of an N atomic system. Since the visualization of the PES is difficult owing to its high dimensionality, a reaction route map (RRM) is occasionally used as a concise representation of PES.[1] RRM is a weighted graph representation of elementary reaction pathways with equilibrium (EQ) and transition-state (TS) geometries on vertices and edges, respectively, with their energies as the weight values. Recently, RRMs can be constructed automatically using GRRM program.[2] Nevertheless, because the layout of the visualization of graphs is arbitrary, extracting the characteristic features of weighted graphs representing RRMs is important for cross-sectional comparison.

In this presentation, we propose a method to extract topological descriptors of a weighted graph based on our *adjusted weight-rank clique filtration* of persistent homology (PH).[3,4] As an example, Fig. 1(b) shows the persistence barcode, invariant descriptors obtained from our method for the RRM of Ag_3Cu_2 depicted in Fig. 1(a). In the presentation, the chemical interpretation of these descriptors will be discussed in detail for metal nanoclusters and small organic systems. Note that the method is related to the work by Mirth *et al.*,[5] where the PH is directly applied to PES. Whereas, our method is more widely applicable to realistic reactions than that.



(a) (b)

Figure 1. (a) RRM of Ag_3Cu_2 and (b) its persistence diagram

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