# Feature Vectorization of Microphase Separated Structures in Polymeric Materials Using Dissipative Particle Dynamics and Persistent Homology for Machine Learning Applications

Yukito Higashi[a], Koji Okuwaki[b,c], Yuji Mochizuki[b,d], Tsuyohiko Fujigaya[a, e,f]*, Koichiro Kato[a,e]*

[a]*Department of Applied Chemistry, Graduate School of Engineering, Kyushu University, 744 Motooka, Nishi-ku, Fukuoka 819-0395, Japan*

[b]*Department of Chemistry and Research Center for Smart Molecules, Faculty of Science, Rikkyo University, 3-34-1 Nishi-ikebukuro, Toshima-ku, Tokyo 171-8501, Japan*

[c]*JSOL Corporation, KUDAN-KAIKAN TERRACE, 1-6-5 Kudan-minami, Chiyoda-ku, Tokyo 102-0074, Japan*

[d]*Institute of Industrial Science, The University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8505, Japan*

[e]*Center for Molecular Systems (CMS), Kyushu University, 744 Motooka, Nishi-ku, Fukuoka 819-0395, Japan*

[f]*International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University, 744 Motooka, Nishi-ku, Fukuoka 819-0395, Japan*

Corresponding authors:

fujigaya.tsuyohiko.948@m.kyushu-u.ac.jp

kato.koichiro.957@m.kyushu-u.ac.jp

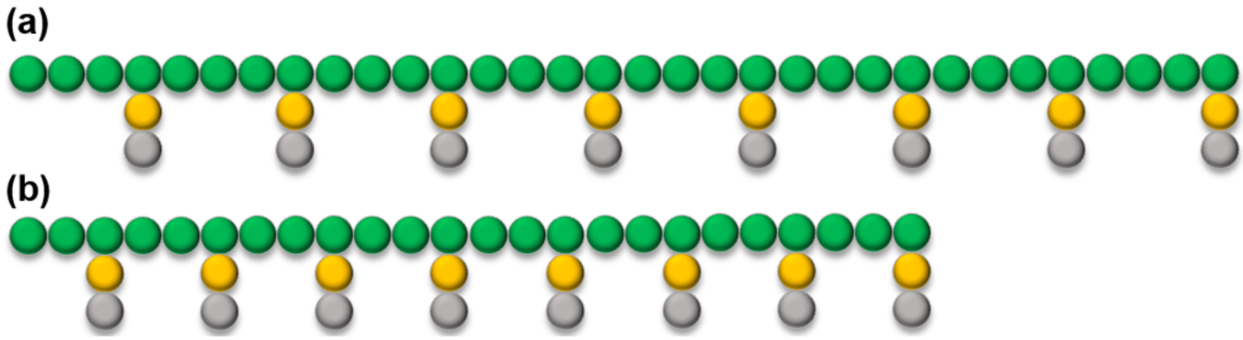


**Figure S1.** The polymer models in this dissipative particle dynamics (DPD) simulation. (a) Nafion and Flemion, (b)Aquivion (green : main-chain, yellow : side-chain root, gray : side-chain terminal).

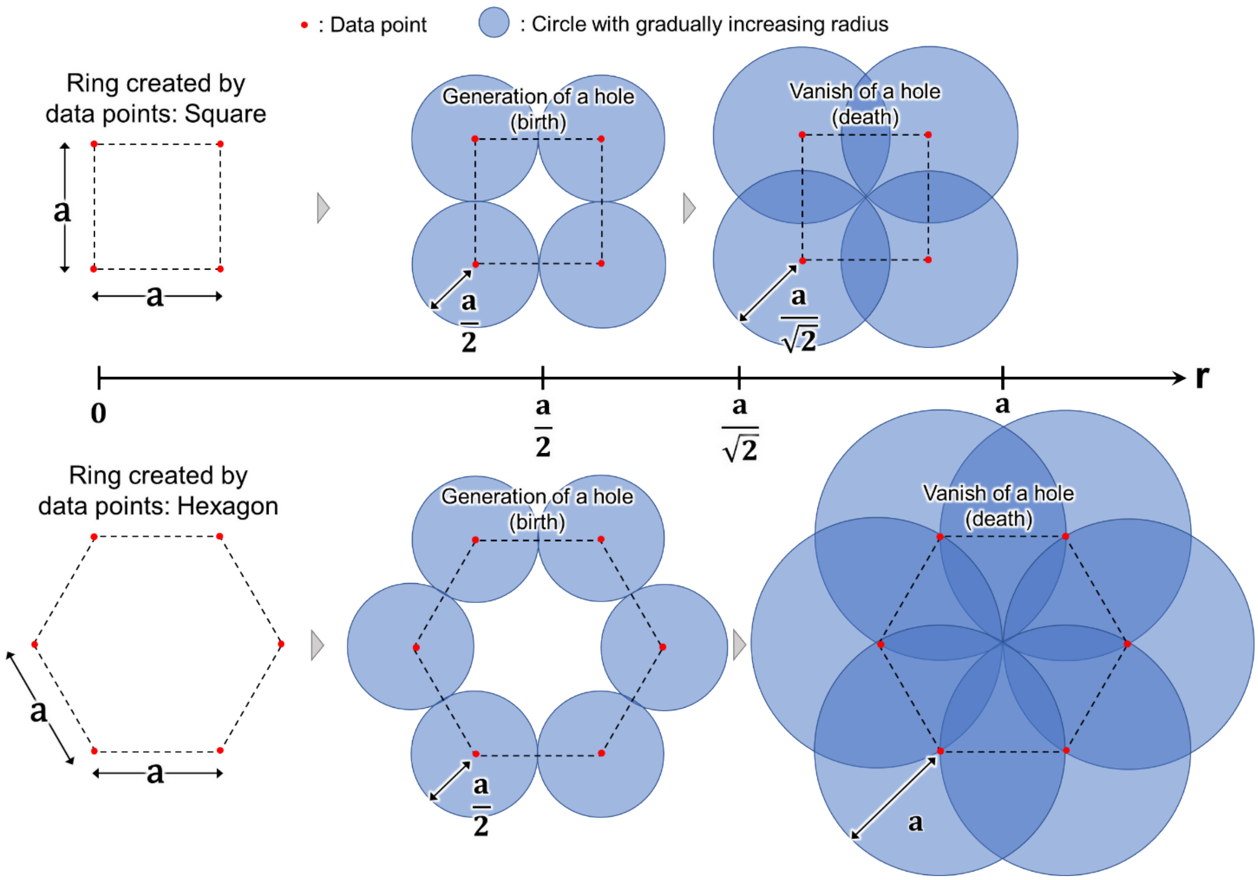


**Figure S2.** Examples illustrate the birth and death radii of a regular polygon, wherein the ring created by the data points is a square in the upper part and a regular hexagon in the lower part. As the circle centered on each data point is gradually enlarged, a hole is created in the center when the radius of the inscribed circle is reached. Upon further enlargement of the circle, the hole in the center disappears (dies) when the radius of the circumscribed circle is reached. Therefore, in the case of a regular polygon, the birth and death radii are the radii of the inscribed and circumscribed circles, respectively.

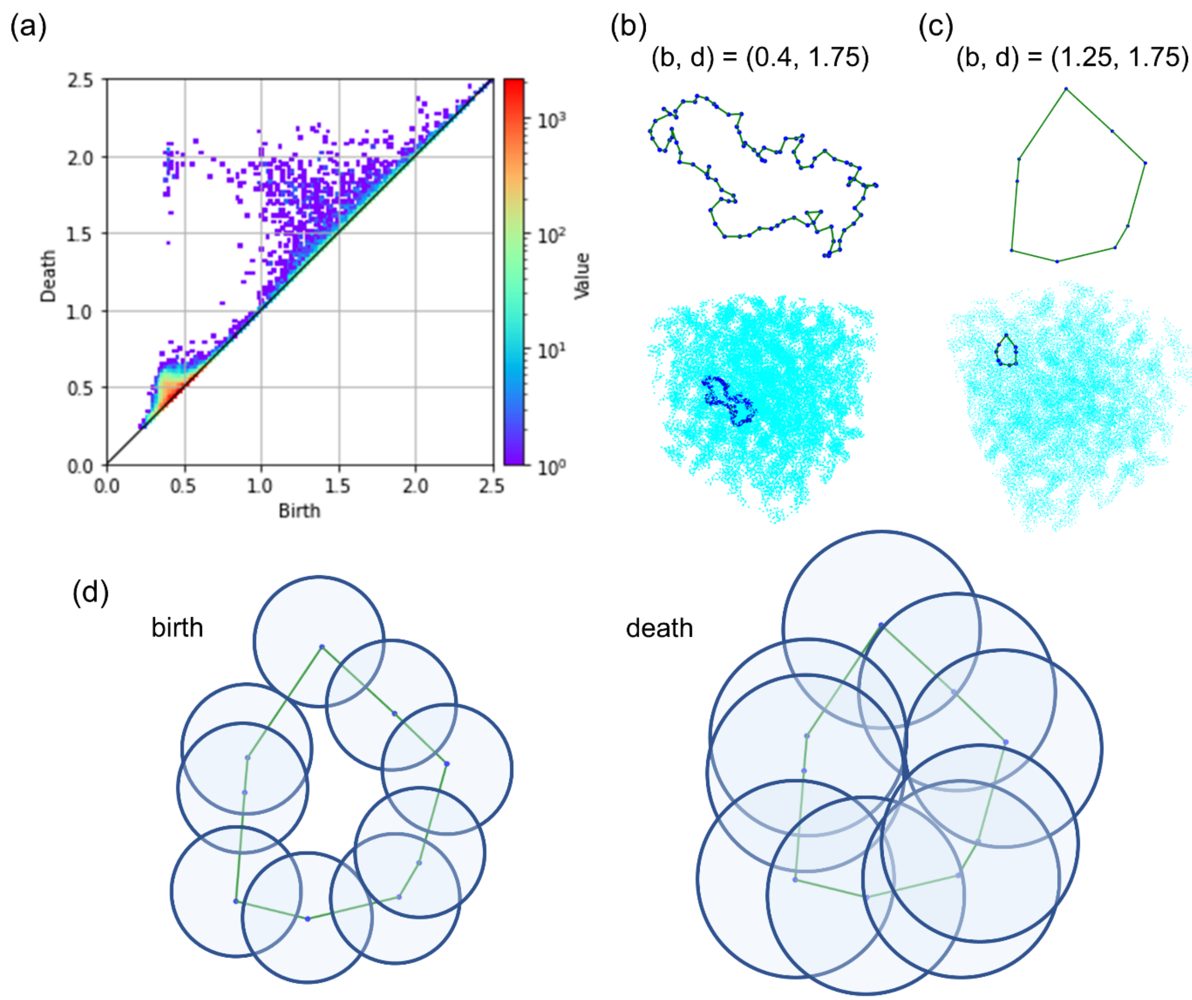


**Figure. S3** (a) Persistence diagram (PD) of water particles in a hydrated polymer membrane, where the color scale represents the density of birth-death pairs. (b, c) Examples of inverse analysis results for selected birth-death pairs from different regions in the PD. The upper panels show the extracted ring structures, while the lower panels display their spatial locations within the full 3D water distribution. (b) A structure with a birth radius of 0.4 and a death radius of 1.75, indicating a smaller-scale enclosed water channel. (c) A structure with a birth radius of 1.25 and a death radius of 1.75, representing a larger-scale enclosed water domain. These analyses provide direct visualization of how persistent topological features correspond to specific structural motifs within the hydrated polymer matrix. (d) Schematic illustration of how such topological features are detected via persistent homology. Blue circles represent virtual spheres centered on each data point. The left panel shows the configuration at the birth radius, where the hole first appears, while the right panel corresponds to the death radius, where the hole is filled in. Although persistent homology is computed using the alpha complex (a subcomplex of the Delaunay triangulation), this depiction provides an intuitive understanding of the geometric scales associated with each feature.

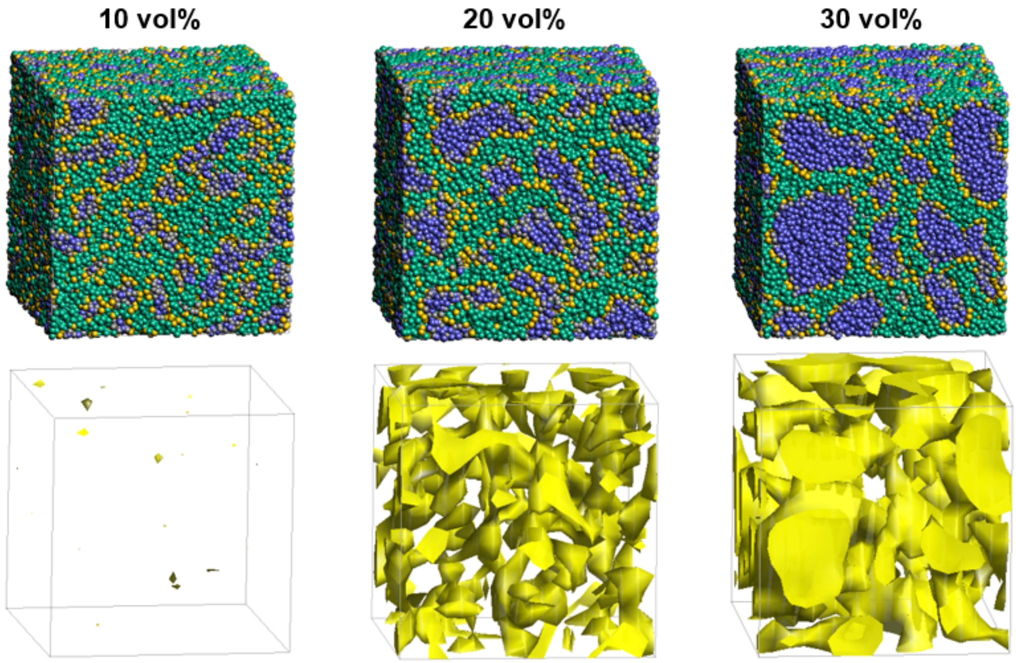


**Figure S4.** Water-content-dependent morphologies (top) and isosurface representation of water particle at density larger than 40 % (bottom) of the hydrated Aquivion membrane system.

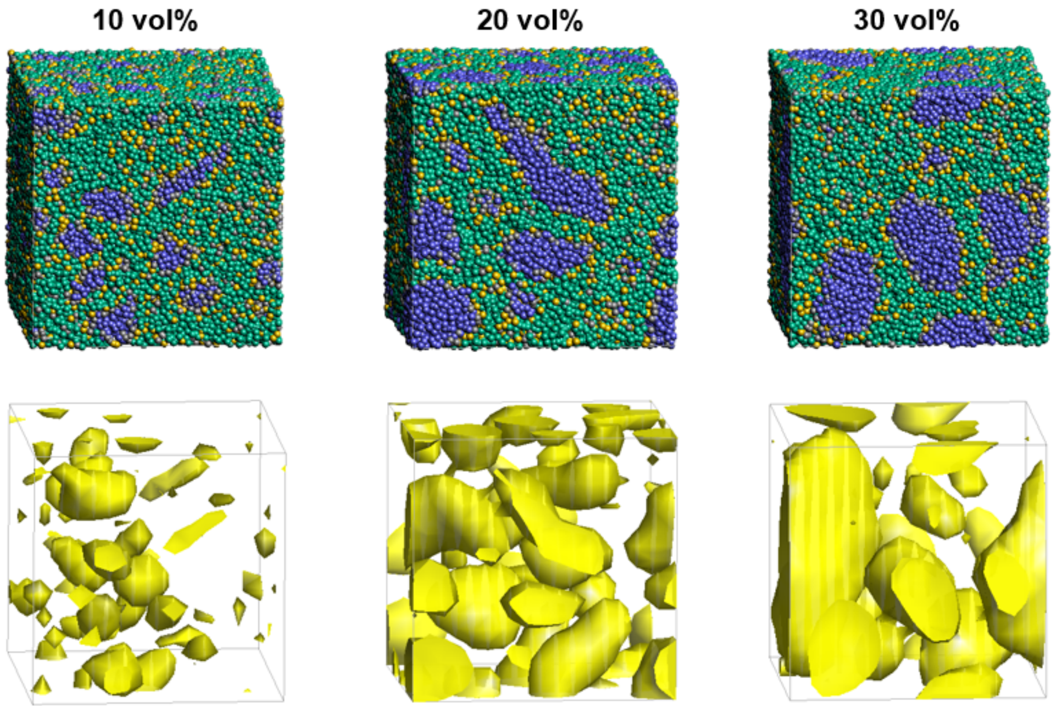


**Figure S5.** Water content dependent morphologies (top) and isosurface representation of water particle at density more than 40 %(bottom) of the hydrated Flemion membrane system.

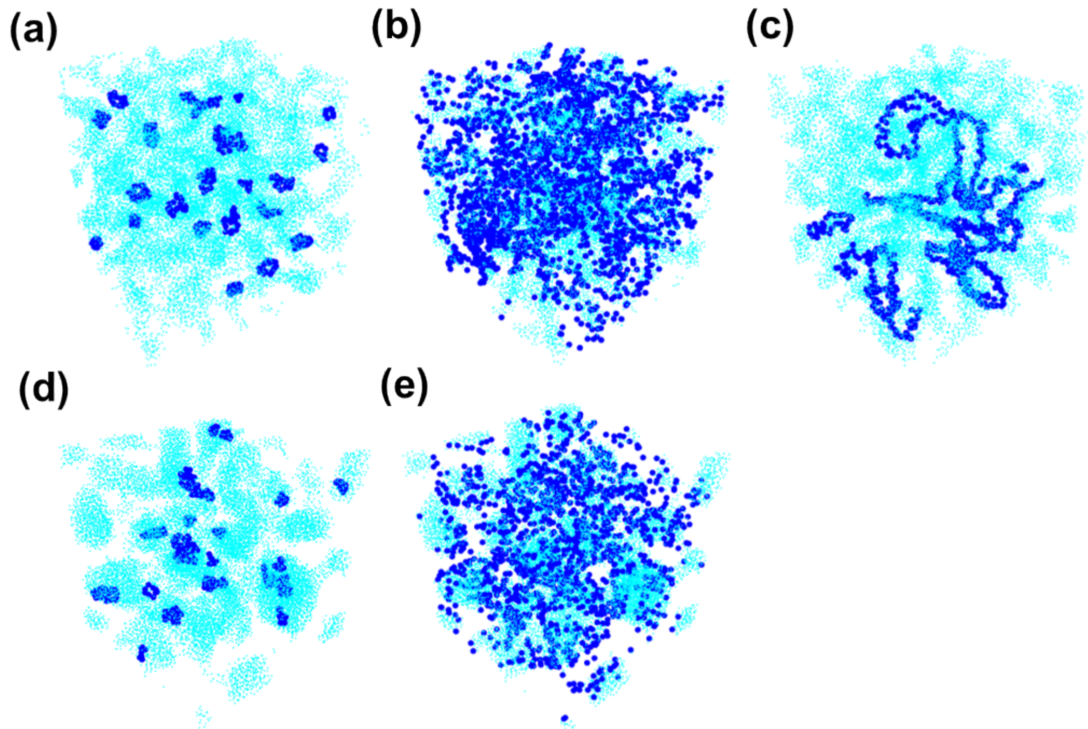


**Figure S6.** Inverse analysis results for PDs of (a-c) Aquivion at 20 vol%, (d, e) Flemion at 20 vol% water content. (a, d: region A. b, e: region B. c: region C.)

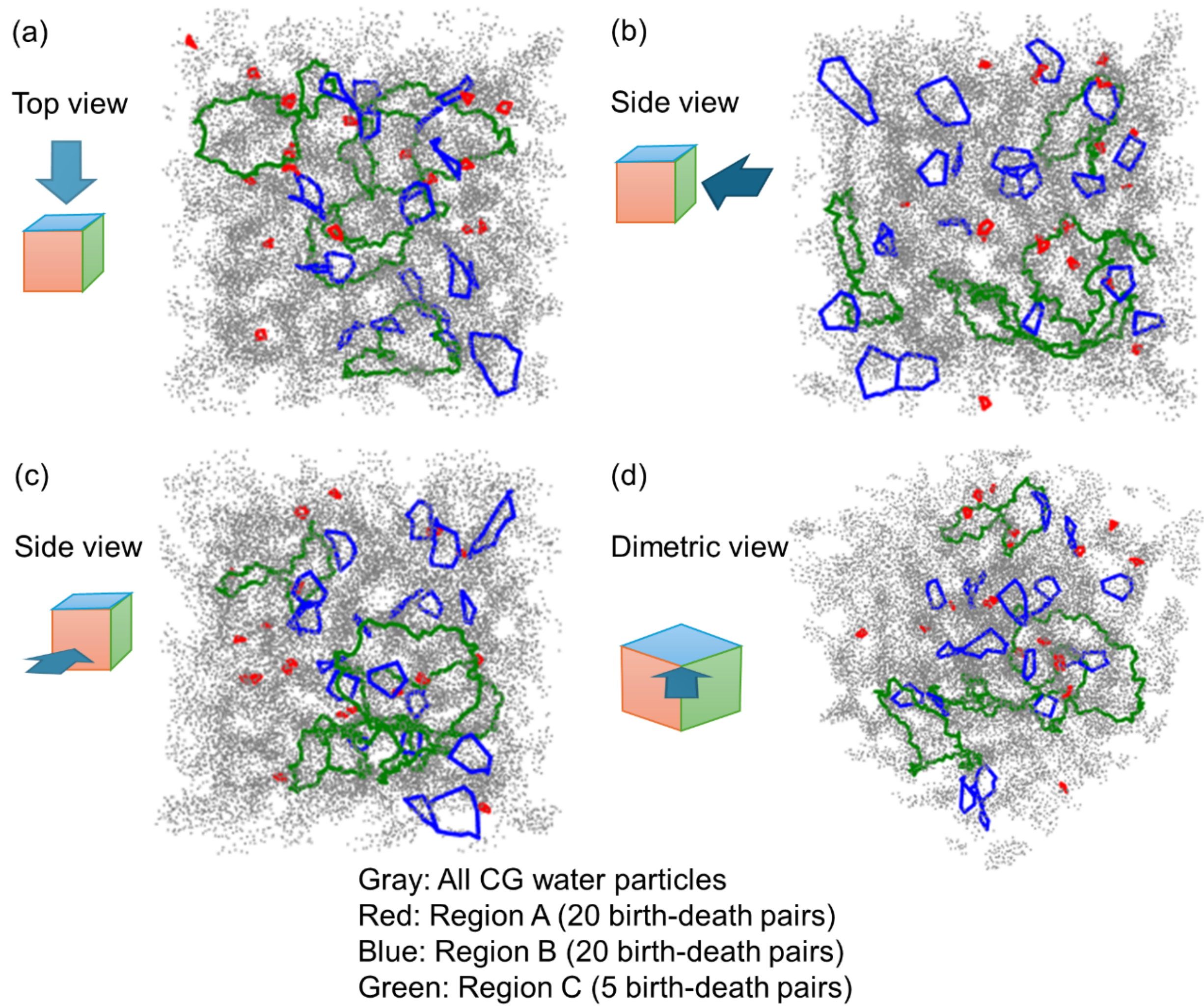


**Figure S7.** Visualization of persistent homology inverse analysis results for Nafion™ at 20 vol% water content. The figure presents different views of the spatial distribution of water particles corresponding to selected birth-death pairs in the persistence diagram. Panel (a) shows the top view, while panels (b) and (c) display different side views, and panel (d) provides a dimetric view for a more comprehensive perspective. The gray dots represent all CG water particles. The red markers indicate water particles extracted from Region A, which consists of 20 birth-death pairs representing small rings sparsely distributed inside the water clusters or channels. The blue markers correspond to water particles extracted from Region B, which includes 20 birth-death pairs corresponding to rings that are spread over the surface of the water clusters and channels. The green markers denote water particles extracted from Region C, which consists of five birth-death pairs forming elongated rings. These elongated rings are indicative of expanded interfaces between water and the polymer, suggesting the formation of water channels that influence water diffusion and proton conduction.

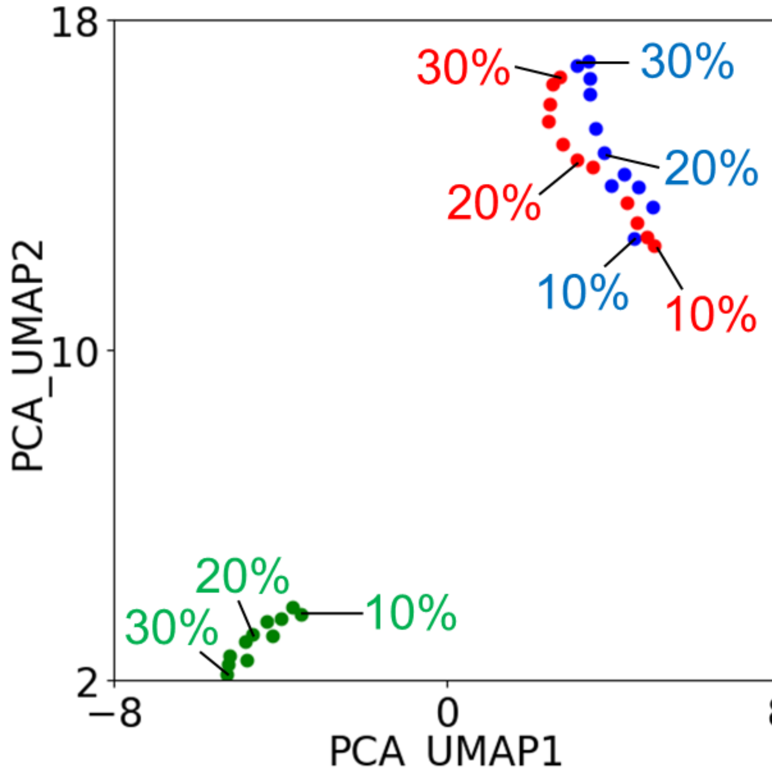


**Figure S8.** Two-dimensional (2D) projection of the PCA-UMAP representation of the persistent homology (PH) features for Nafion™ (red), Aquivion® (blue), and Flemion™ (green) at different water contents (10–30 vol%). The horizontal and vertical axes correspond to the first and second PCA-UMAP components, respectively. The distribution of data points in 2D preserves the relative positions of different polymers and their water content trends, similar to the 3D representation. However, as discussed in the main text, the third dimension (PCA-UMAP3) captures additional structural variations that correlate with water diffusivity and proton conductivity. Therefore, the 3D representation was used in the primary analysis.