Persistent homology characterization

Topology based characterization

Method:

Input descriptors:

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[**3D coordinates of the data points representing the Si structures**]

Point cloud

Neighborhood calculation:

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[**Neighborhood Calculation: For each point in the input dataset, the neighborhood, defined by a radius or distance parameter is calculated. Points within this radius are considered neighbors of the central point.**]

Simplex Construction:

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[**Based on the neighborhoods, complex simplices of varying dimensions are constructed.**]

Barcode Construction:

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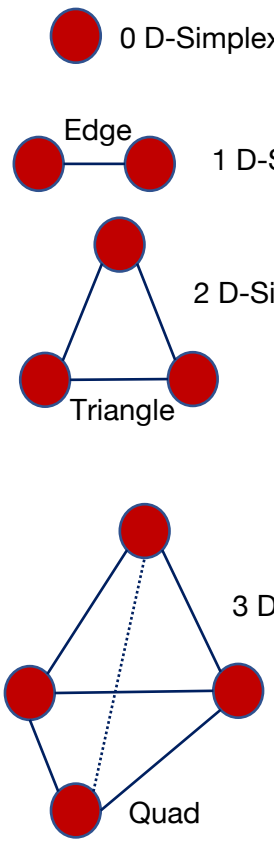
[**Based on the filtration parameter used in the construction of the simplicial complex which indicate the ordering of the construction of the simplicial complex, the barcode is constructed for different structures. This parameter determines the sequence in which simplices are added to the complex, influencing the topological features observed.**]

Explanations:

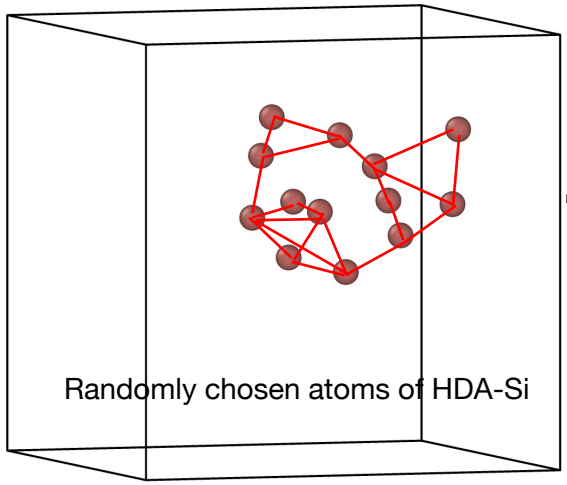
Simplex Construction:

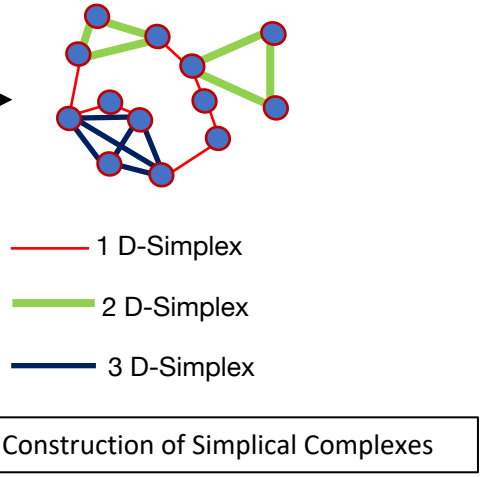


f(α)

Taken as central atom.

The f(α) gradually builds up as higher-dimensional simplices are added to form simplical complexes.





Construction of Simplical Complexes

Topological features captured by the higher dimension data derived from simplices are:

1. **Connected Components [0 dimension]**
2. **Holes [2 dimension]**
3. **Tunnels [2 dimension]**
4. **Cycles[1 dimension]**
5. **Cavities [2 dimension]**

These are based on the filtration parameter[ε] of the complex α, is chosen by default based on the characteristics of the data.
The default behavior aims to capture the geometric structure of the point cloud effectively.

Persistence Diagram and Barcode Construction

Now we have the topology features to represent the structure based on the filtration parameter. Then we compute the persistence intervals for each structure and compute the barcode.
(Explained in next slides)

Persistence Diagram Construction:

Primary Concepts of Homology Persistent Representation of structures:

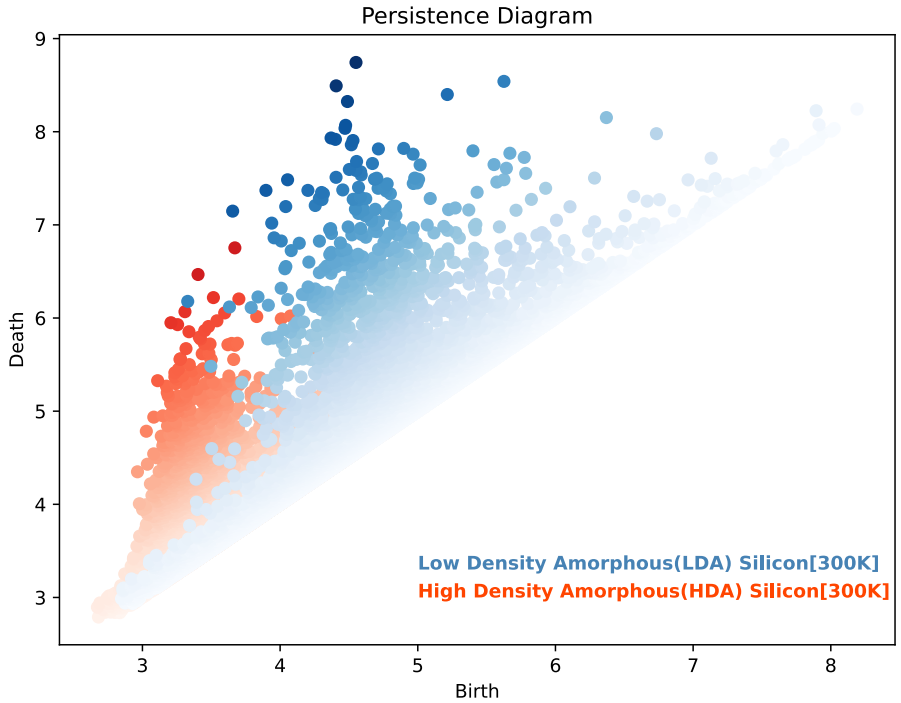
Birth: Filtration value(ε) when the topological feature[based on the dimension you choose] first appears.
Example: If the topology dimension is chosen as 2, the birth is when a hole first appears.

Death: Filtration value(ε) when the selected topological feature[based on the dimension you choose] disappears.
Example: When the hole that started disappears.
The intervals of birth and death is called **Persistence Interval.** That means each interval captures the birth and death of a topological feature based on what dimension feature you choose.

Example

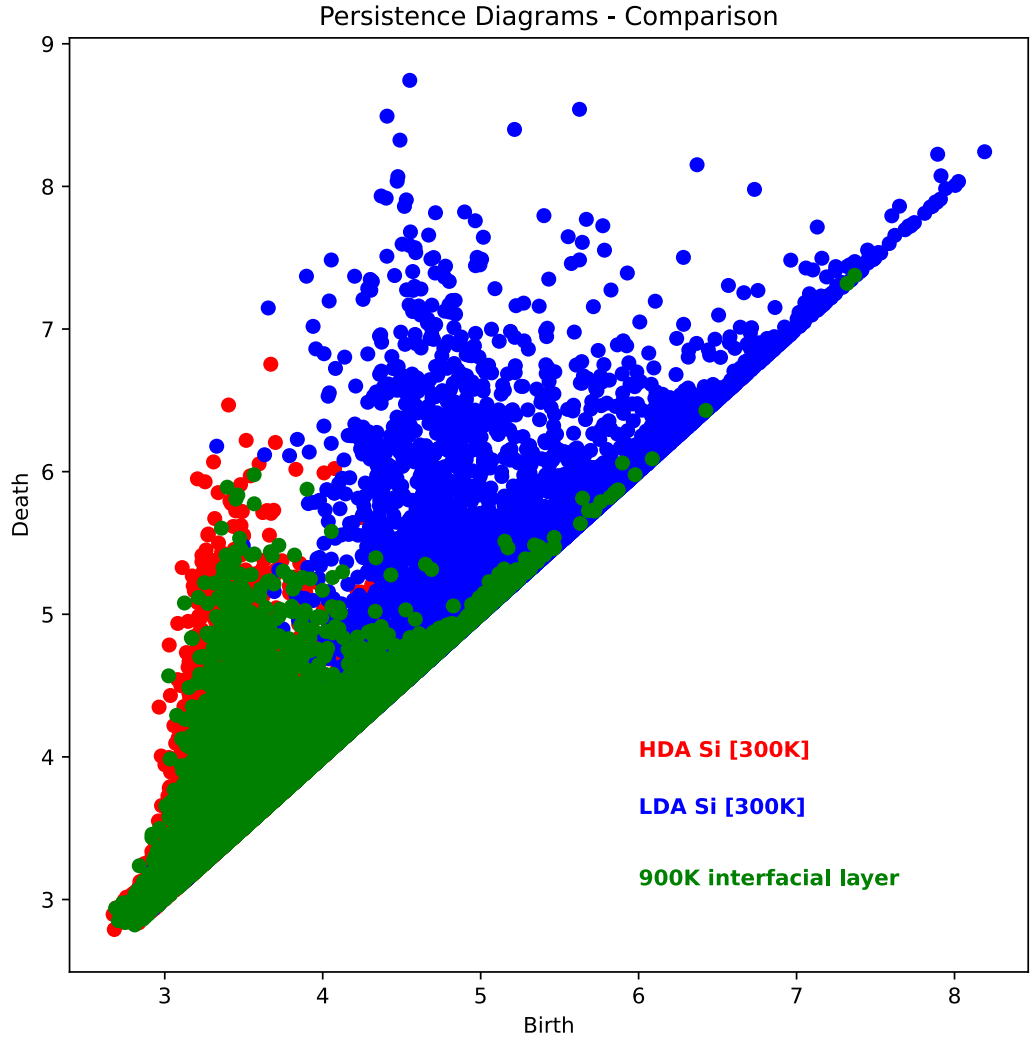
Suppose the filtration parameter is chosen to be Euclidean distance between two point in the point cloud.
In a denser structure, intervals between the birth and death of a void should be small. That means the persistence interval for a specific filtration value, is smaller if compared to the less dense structures.

This concept of Persistence Interval is portrayed in the diagram which are called Persistence Interval Diagrams. The diagrams are a function of birth and death of the topological feature.



In this figure, the topological feature dimension is chosen as 2D.
The HDA-Si (represented by reds), has lower persistence values when compared with LDA-Si(represented by blues), for similar dimension of topological features.
This is because interval of birth and death between the 2D features such as voids, tunnels are less in HDA because of closely packed atoms. Whereas the intervals between birth and death of 2 dimensional topological features in LDA, is larger.

Persistence Diagram Comparison:



In this figure, we compare the structures of HDA-Si, LDA-Si and time evolved interfacial structure at 900K with P_N = 12GPa. The interfacial structure is formed when cu-Si is slid over LDA with a sliding velocity of 0.1m/s.

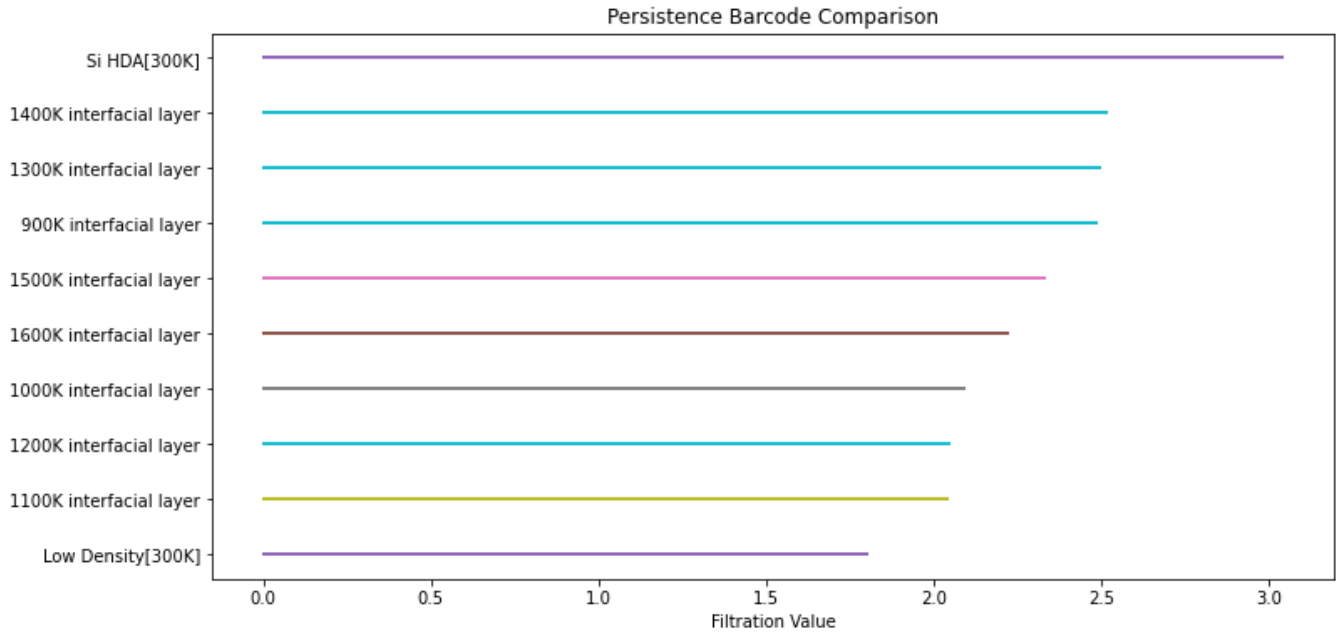
The topological feature dimension is chosen as 2D. Now based on the explanation provided in previous slide, we see that for both the interfacial structure and HDA-Si, the persistence interval is less compared with that of LDA-Si. In other words, for interfacial structure and HDA, the 2D topology features appears and disappears faster when compared to LDA-Si.

So, based on topological features, the interfacial layer formed at 900K, is similar to the HDA Si structure.

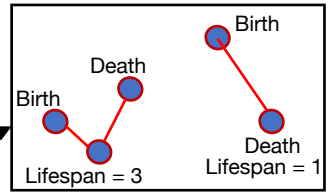
Barcode Construction [0D topological features]:

What if we choose the topology to be 0D which means the interval values will take the information of features like connected components. In other words, only 1D simplex are considered.

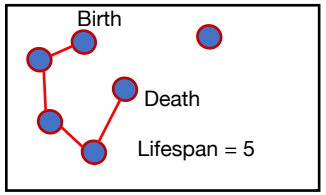
The barcode represents the persistence or lifespan of a particular feature.
For filtration value 0, i.e., the bottom-end of the line segment is the birth of a feature, and the higher end is the death of a particular feature.
Longer the line segment, the persistence of that feature is higher.



In this figure, only 1D simplex are considered which are the connecting components between 2 vertices.
The LDA-Si has lower lifespan when 0D topological features are considered. **Because there are more voids or gaps between two atoms, the lifespan of a connecting component is small within the filtration component such as Euclidean distance**. The voids and cavities are not considered here.
But for higher densities and compressed structures, the persistence is larger.



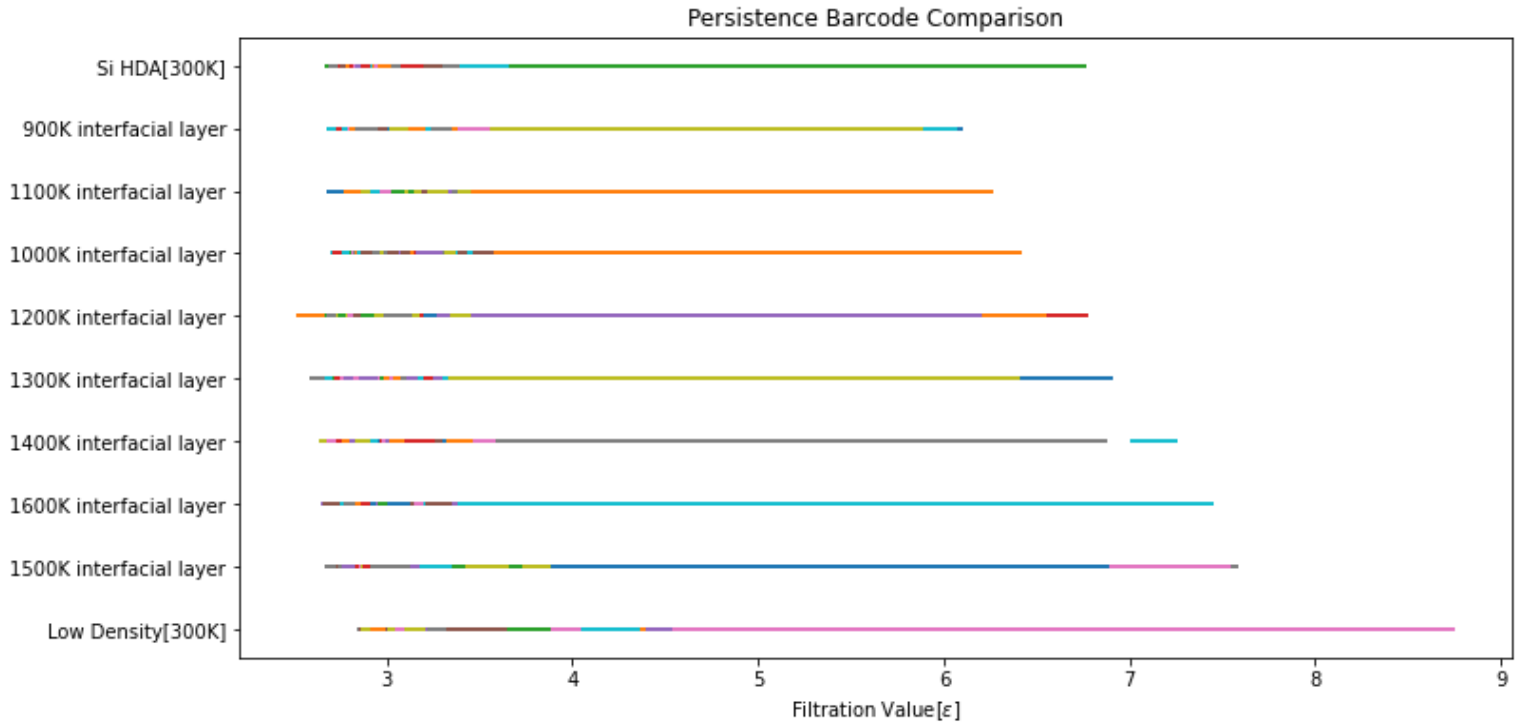
LDA-Si schematic



HDA-Si schematic

Barcode Construction [2D topological features]:

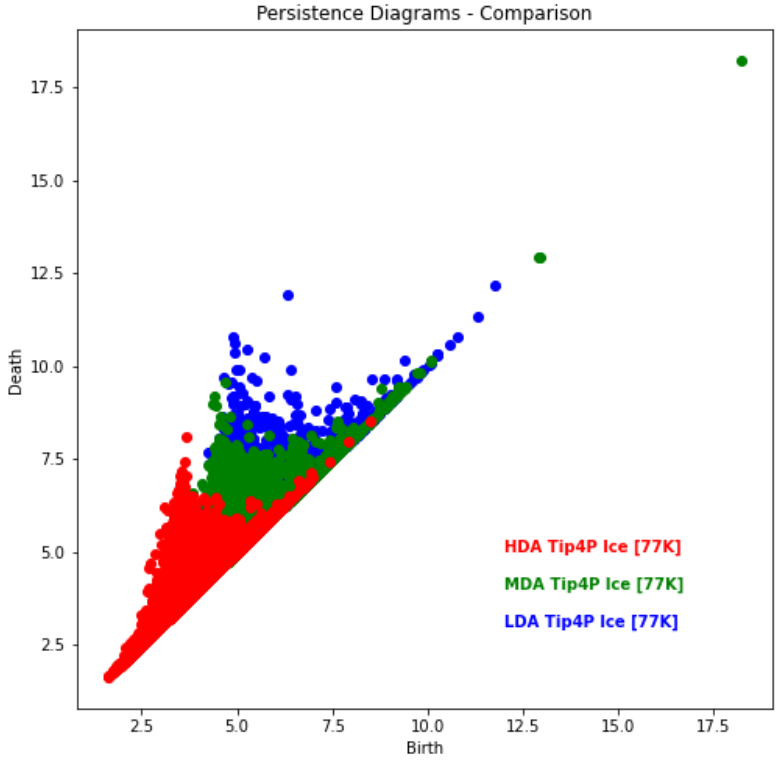
As explained previously, the 2D topological features comprises of loops, voids, cycles, etc. So, this slide will show a similar persistence value as shown in persistence interval diagram. But it will be represented by barcode.

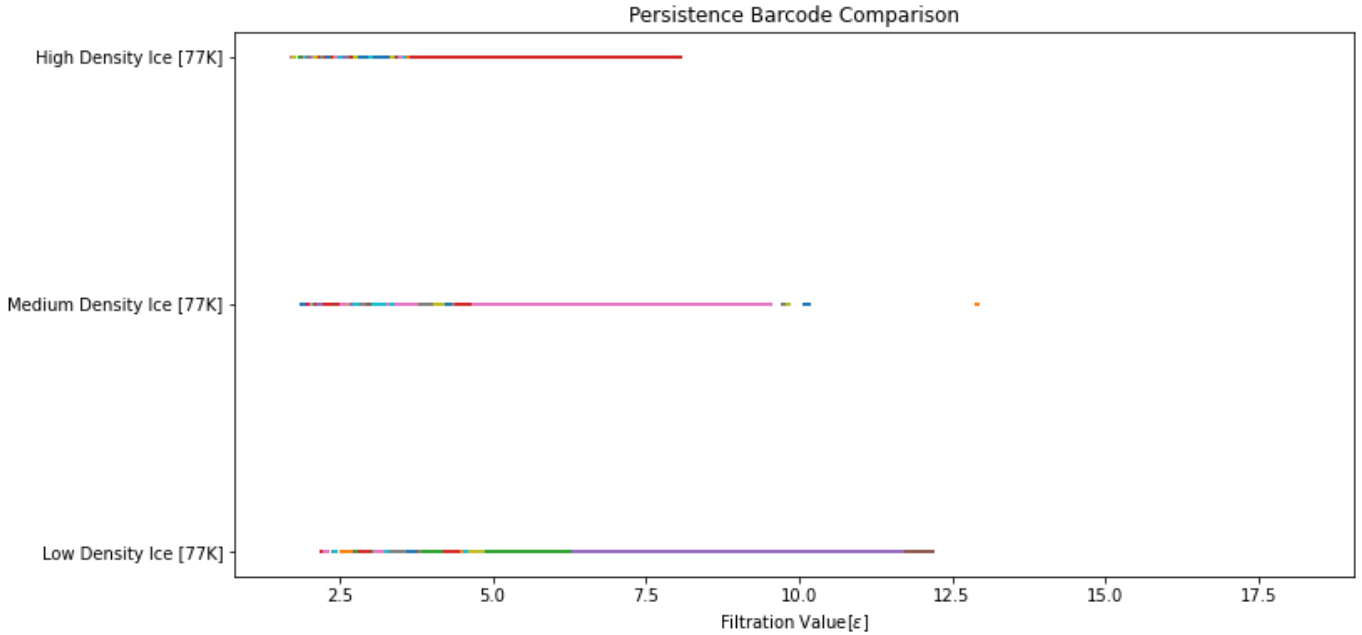


In the above figure, 2D topology features such as loops, voids, tunnels are considered.

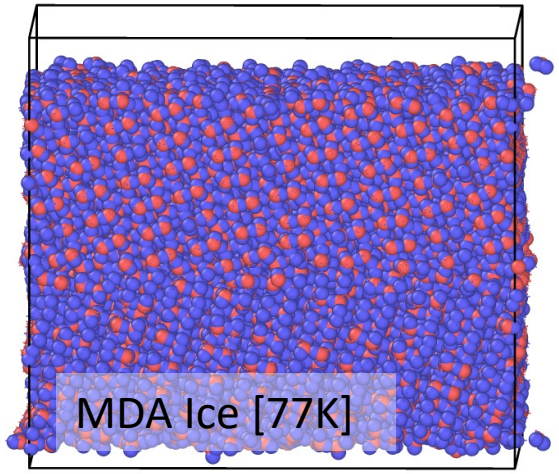
- In LDA-Si, the bottom-end of the line segment, starts at a higher value of ε. This means the 2D features in LDA starts at a higher filtration value.
- The different colors of a line segment represent different topological features and their corresponding persistence. **The starting of a color marks the birth of a feature and end is the death of a feature.**
- The gap in the line segment for interfacial layer at 1400K, implies that a feature has died but the next feature has not yet started.
- The longer the line segment, the more persistent the features are. For example, if holes are considered as one of the topological feature. The interval between birth and death of a hole is more persistent in LDA-Si, than in HDA-Si.
- **The lifespan of a 2D topological feature like, holes, cycles, loops, etc, are larger in low density structures than in high density structures.**

Persistence Diagram and Persistence Barcode Comparison:





Although the persistence interval of MDA ice is in between the LDA and HDA ice, because of the 2 water molecules that are far from the rest of the structure, the features start and end at a higher value of persistence



Explanation for gap in the line-segment:

As stated before, the gap in the line segment signifies that a topological feature did not start until a higher filtration value.

In the MDA ice structure, there are 2 water molecules which are far from rest of the atoms. That is why there is a gap in the MDA ice.