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Revealing Structural Features of Amorphous Monolayer Carbon Using Persistent Homology Analysis

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Amorphous Monolayer Carbon (AMC), a disordered form of graphene first synthesised in 2020, displays high flexibility but has low mechanical strength, restricting potential application in areas such as flexible electronics.

Existing descriptions of 2D amorphous materials generally fall between assigning materials to Zachariasen continuous random networks, as frequently ascribed to bulk amorphous materials, or to the crystallite model - but a universal framework is not yet present. Since AMC does not possess obvious order, it cannot be characterised using approaches relying on unit cells, such as Monte Carlo techniques.

Some promise lies in recently synthesised forms of AMC with particular distributions of local “graphene-like” nano-crystallite areas. Nano-crystallite forms of AMC have been shown to maintain AMC’s flexibility, while adding graphene-like strength. However a general understanding has not been obtained.

To address this, we apply Persistent Homology to atomic configuration data of AMC. This method allows computation of topological features of a space, persisting across length scales. Features remaining present after performing Persistent Homology are more likely to represent features of the underlying space, potentially revealing previously obscured features.

Our approach gives both insight into the structural and mechanical properties of AMC, in addition to gaining general insight into amorphous 2D materials. Understanding of hidden order may allow strategies in design and synthesis of amorphous materials in such a way that maintains strength and flexibility, to reconcile gaps between theory and implementation. This approach underscores the potential of topological data analysis to add universality to materials science as a whole, on a pathway to technological evolution.

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