Amorphous carbon materials – experiments and computational studies augmented by machine learning

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Amorphous carbon thin films have extraordinary properties that make them attractive for many applications ranging from protective thin film coatings to electrochemical biosensors. Tetrahedral amorphous carbon (ta-C) is a special form of a-C characterized by its high sp^3 bonded carbon content. During recent years, we have studied in depth structural, electrical and electrochemical properties of ta-C and a-C thin film structures using a wide variety of sophisticated experimental techniques. However, these results do not provide us atomic level insight behind the observed behavior. In this presentation, we will show how a combination of computational studies augmented by machine learning approaches and experimental results can be used to understand the origin of material properties of amorphous carbon at the atomic level. Moreover, several open questions related to interpretation of experimental data that would highly benefit from various computational approaches are identified for future work.