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Hydrogen bond networks in Graphene Oxide Composites: Structure and Mechanical Properties NIKHIL MEDHEKAR, VIVEK SHENOY, Brown University — A composite structure made of several layers of graphene oxide has drawn a considerable attention as a paper-like composite material due to its excellent electronic and mechanical properties. Using molecular dynamics simulations, we study the atomic-level structure of such multilayer graphene oxide composites. We find that in these structures, the individual graphene oxide layers are interlinked via a non-uniform network of hydrogen bonds mediated through oxygen-containing functional groups and water molecules. Based on a quantitative analysis of hydrogen bond networks, we show that they play a crucial role in determining the overall morphology of graphene oxide composites. The predicted structural and mechanical properties are in good agreement with experimental observations.

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