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Atomistics of carbon nanotube-polyacrylonitrile interfaces for next-generation carbon fibers: A multiscale computational study JUHO LEE, JI IL CHOI, Graduate School of Energy, Environment, Water, and Sustainability (EEWS), Korea Advanced Institute of Science and Technology, Daejeon, 305-701, Korea, SEUNG SOON JANG, SATISH KUMAR, Department of Materials Science and Engineering, Georgia institute of Technology, Atlanta, 771 Ferst Drive, GA, USA, ART E. CHO[1], Department of bioinformatics, Korea University, Sejong, 339-700, Korea, YONG-HOON KIM[2], Graduate School of Energy, Environment, Water, and Sustainability (EEWS), Korea Advanced Institute of Science and Technology, Daejeon, 305-701, Korea — Atomic-scale understanding of the carbon nanotube (CNT) – polyacrylonitrile (PAN) interfaces is a critical missing element for the development of next-generation carbon fibers. In this presentation, we provide the systematic atomistic analyses of the CNT-PAN interfaces based on a multiscale computational approach combining density-functional theory (DFT) and force-fields molecular dynamics (FFMD) simulations. Based on DFT calculations, we identify the preferable CNT-PAN configurations and furthermore elucidate the electronic origin of the CNT-PAN binding. Next, via FFMD simulations, we extract more realistic large-scale interfacial CNT-PAN atomic configurations and confirm that they faithfully reflect the geometric motives identified in DFT calculations. Implications of our findings in the context of development of advanced carbon fibers will be discussed.

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