Computer simulation identifies a key principle for next-generation carbon fibers

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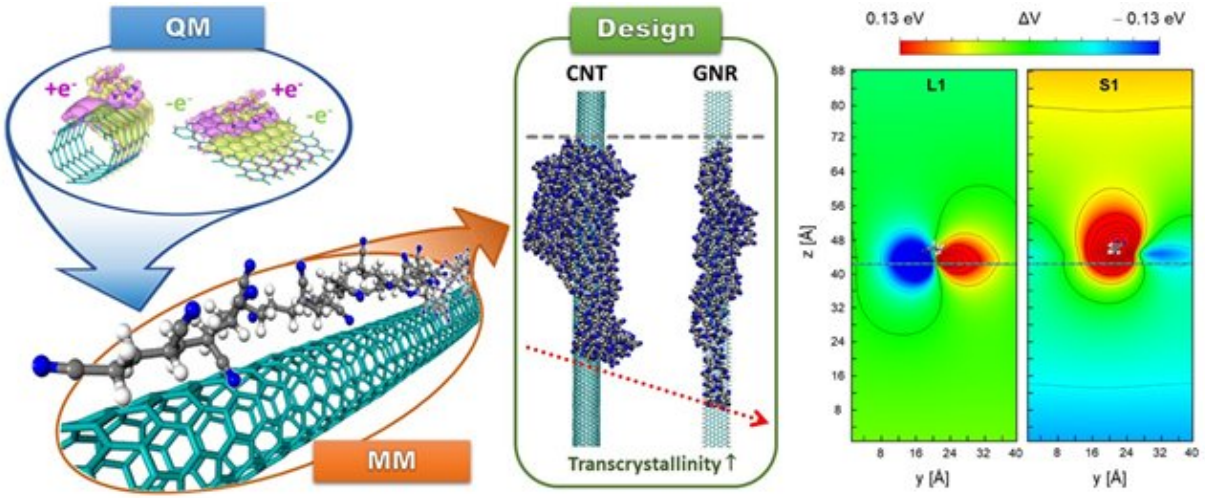

Credit: Korea Advanced Institute of Science and Technology

Performing state-of-the-art computer simulations, a KAIST research team identified an atomistic design principle to produce high-quality, next-generation carbon fibers.

Carbon fibers are light-weight yet excellent in mechanical strength and thermal resistance. Boasting these properties, they can be diversely applied in high-technology sectors, including automotive, aerospace, and nuclear engineering.

They are produced from a polymer precursor through a series of spinning, stabilization, and carbonization processes. However, there is a major obstacle to producing high-quality carbon fibers. That is, when there exist ill-defined regions within the polymer matrices, they result in disorder and defects within the produced carbon fibers.

As a solution to this problem, it was proposed that the introduction of carbon nanotubes (CNT) could enhance polymer orientation and crystallization. However, although the alignment geometry of the CNT-polymer interface apparently affects the quality of produced fibers, the atomistic understanding of the CNT-polymer interface has so far been lacking, hindering further developments.

To clarify the nature of CNT-polymer interactions, Professor Yong-Hoon Kim from the Graduate School of Energy, Environment, Water and Sustainability and his team employed a multiscale approach that combines first-principles density functional theory (DFT) calculations and force-fields molecular dynamics (MD) simulations and revealed the unique structural and electronic characteristics of polymer-CNT interfaces.

Here, they studied polyacrylonitrile (PAN)-CNT hybrid structures as a representative case of polymer-CNT composites. PAN is the most common polymer precursor, taking more than 90 percent of carbon fiber production.

Based on their DFT calculations, the team showed that the lying-down PAN configurations give a larger PAN-CNT binding energy than their standing-up counterparts. Moreover, maximizing the lying-down PAN configuration was shown to allow linear alignments of PANs on CNT, enabling the desirable ordered long-range PAN-PAN packing.

They also identified the CNT curvature as another significant factor,

giving the largest PAN-CNT binding energy in the zero-curvature graphene limit. Conducting large-scale MD simulations, they then demonstrated that graphene nanoribbons are a promising carbon nano-reinforcement candidate by explicitly showing its strong propensity to induce linear alignments of PANs adsorbed on them.

Professor Kim said, "This research can be an exemplary case where the quantum mechanical simulations identify basic principles for developing advanced materials. Computer simulation studies will play a greater role thanks to the advances in the simulation theory and computer performance."

More information: Juho Lee et al. Origin and Control of Polyacrylonitrile Alignments on Carbon Nanotubes and Graphene Nanoribbons, *Advanced Functional Materials* (2018). DOI: 10.1002/adfm.201706970

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