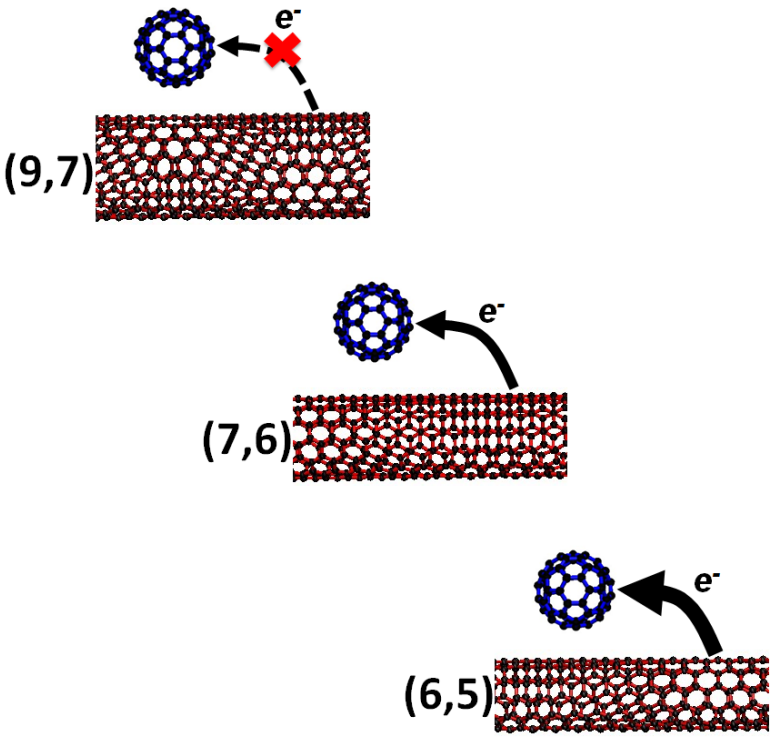
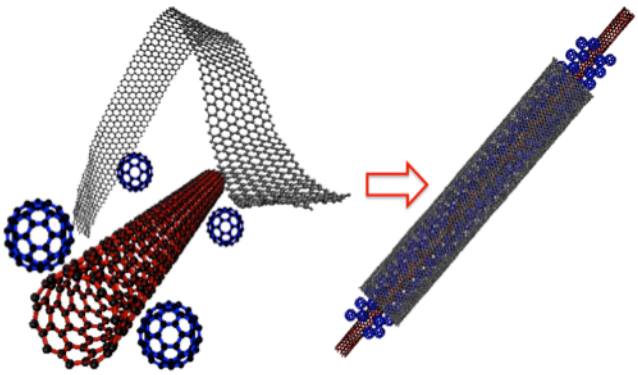
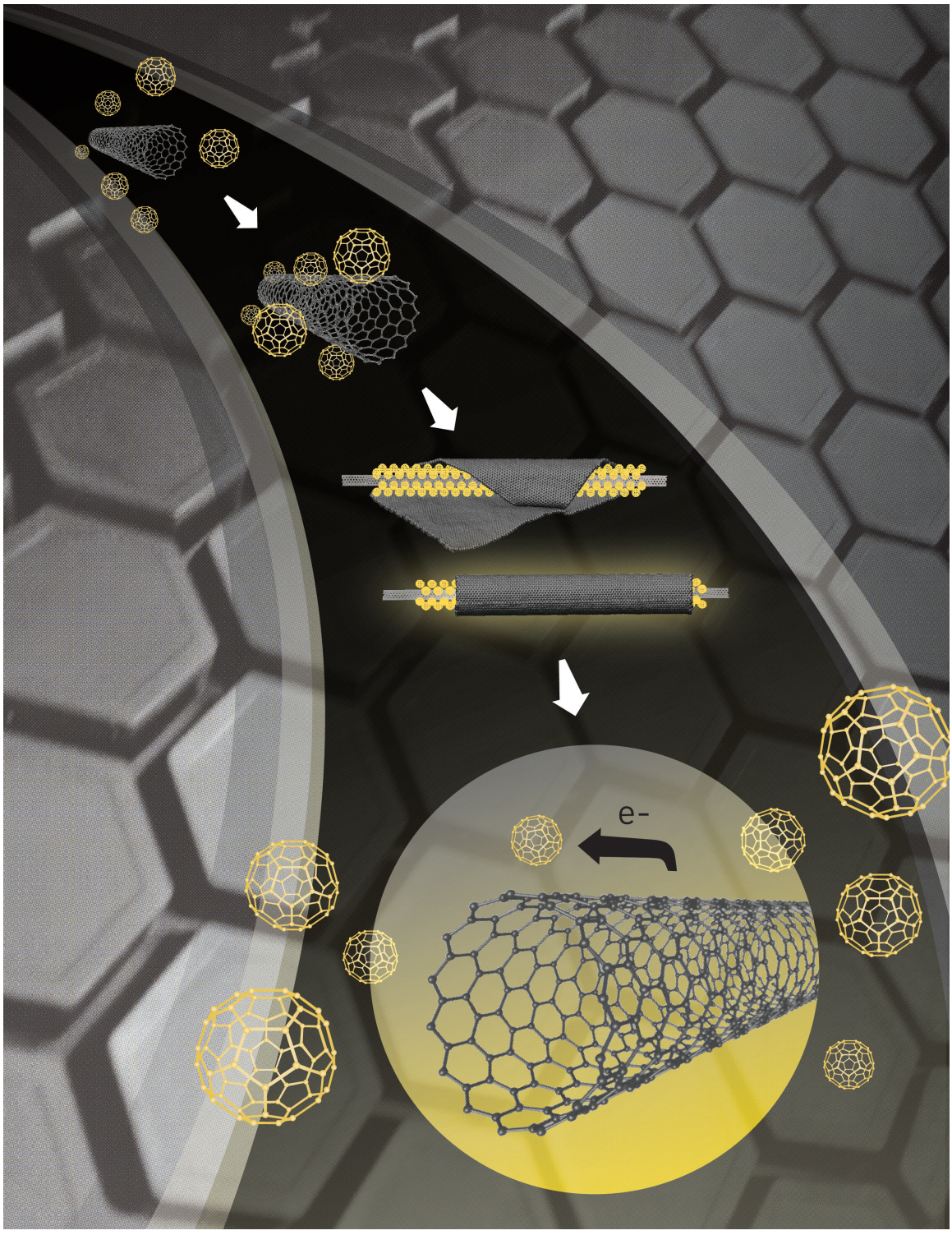
First Principles Study of the Electronic Properties of Nanocarbon Materials for Photovoltaics. Recently, nanocarbon materials (graphene, carbon nanotubes, fullerenes) have been shown to have promising charge transport properties, making them a potential new architecture for photovoltaics. This project will model the electronic structure and electron dynamics of these nanocarbon composite materials using quantum chemistry methods such as density functional theory. In particular, we will examine the role of the number and location of the fullerenes adsorbed along the carbon nanotube in the electron transfer process and compare the behavior of C_{60} and less-symmetric C_{70} fullerenes. Later stages of the project will analyze the charge transport through the graphene layer.



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