Chain Length Dependent Structural Properties of Alkylated Graphene Oxides.

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Graphene oxides(GOs) and their derivatives were widely studied but their chemical composition or structure were not completely known yet. The relation between nano-scale chemical structure and bulk property was examined by molecular simulations combining two different methods. Realistic modelling of GO and alkylated graphene oxide(AGO) were abled considering formation energy of oxidation groups and adsorption process of alkyl amines using grand canonical monte carlo (GCMC) simulation. Molecular dynamics simulation was also conducted on layered AGOs with chemical formula decided from the modelling to analyze the alkyl chain length effects on AGO properties. The structural properties showed transition point according to chain length which also observed by experiments which could give guide to control material property of AGOs.