Atomistic Modeling of Thermochemical Processes for Efficient Recycling of Polymer Composite Materials

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The investigation of novel solvolysis methods for recycling carbon fiber-reinforced polymers is gaining increasing attention, primarily driven by the high environmental impact of composite materials used in various industrial sectors, such as wind energy. Nevertheless, solvolysis relies on the coupling of physicochemical and heat&mass transfer phenomena occurring over multiple scales, so a mechanistic understanding of the process has not yet been achieved. In this context, nanoscale modeling and atomistic simulations can provide useful insights into the interactions and interface properties of composite materials.

The aim of this work is to develop a suitable simulation protocol based on molecular dynamics to help in understanding the mechanisms underlying these recycling processes and thus assist in the selection of appropriate thermodynamic parameters, with a specific emphasis on supercritical solvolysis. First, different water models are employed and compared to explore the properties of water under supercritical conditions, since supercritical water has great potential as a reaction medium. Then, some representative polymer models are built through the development of specific algorithms, with the purpose of generating realistic polymer networks and accurately replicating their experimental properties. Next, atomistic models of epoxy-based composites will be assembled and analyzed to explore the interface interactions between matrix and fillers. Simulations of solvent infiltration into the composite material will then be conducted, and the heat&mass transfer phenomena occurring at composite-solvent interfaces will be investigated. The incorporation of reactive force fields and other innovative computational approaches into the simulation flow will also be considered, thus enabling a more detailed analysis of the chemical processes involved in solvolysis.

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