577c Structure and Dynamics of Dendrimer Encapsulated Nanoparticles in Aqueous Solutions

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Nanoparticles are targeted as superior materials for catalytic applications. Their synthesis done in solution of templates and stabilizers such as polymers and surfactants has become an important topic due to its potential to prevent particle sintering. If the active sites of the nanoparticles are available for reaction, then the system stabilizer-nanoparticle may be a good candidate for homogeneous catalysis whereas removal of the stabilizer would be required for heterogeneous catalysis. For instead, dendrimers have proven good not only as templates but also as hosts. The current view is that nanoparticles lie in the interior voids of dendrimers and remain stable there. Consequently they may not aggregate to other nanoparticles although intradendrimer and interdendrimer aggregation have been postulated. Therefore an understanding of the dynamics of the system stabilizer-nanoparticle could help to elucidate the stabilizing role of dendrimers and test their ability as stabilizers against agglomeration. We perform molecular dynamics simulation to follow the interaction between two dendrimer encapsulated nanoparticles (DENs) in presence of water as solvent. Dendrimer and cluster dynamics are recorded and analyzed accordingly.