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Novel structure formation of dipolar Janus particles (JP) in electrolytes: A molecular dynamic (MD) simulation study MAHDY MALEKZADEH, BAMIN KHOMAMI, Materials Research and Innovative Laboratory (MRAIL), Department of Chemical and Biomolecular Engineering, University of Tennessee, Knoxville — There have been tremendous number of experimental studies and number of simulations in recent years trying to elucidate the underlying principals which determine structure formation of colloidal systems of JP. However most of simulations utilize relatively simple models and lack inclusion of long range columbic interactions. In this work MD simulations have been performed to understand effects of surface charge density and volume fraction (0.01-0.17) on structure formation and radial pair distribution function (RDF) of JPs of 6 nm in diameter with opposite charges on each hemisphere. Inclusion of long range columbic interaction via Ewald summation leads to formation of novel structures such as rings, chains and layered large spheres (about hundreds of nanometers) in accord to experimental observations. Moreover based on possibility of defect formation during synthesis, defects were introduced into each JP by slightly altering the uniform charge distribution on each hemisphere. Our results show in presence of small amount of defects (<10%) no significant changes occur in RDF, however increasing defect sites up to around 20% will significantly changes structure formation and combination of aforementioned structures concur to SFM and SEM images.

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