Abstract Submitted for the MAR12 Meeting of The American Physical Society

Novel building blocks for materials by design: Janus particles and other patchy colloids<sup>1</sup> RIGOBERTO HERNANDEZ, MATTHEW C. HAGY, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA 30332-0400 — The emergent assembly of nonisotropically structured colloidal particles can lead to novel materials with requisite optical or mechanical properties. We have developed two models—one that includes detailed interactions between particles and another that coarse-grains the interactions—so as to explore the equilibrium and dynamics effected by varying interaction heterogeneities. In particular, we have performed a series of simulations of systems consisting of Janus particlesin which each of two hemispheres can be characterized by a single interaction type such as charge or degree of hydrophobicity. The equilibrium structure of Janus clusters has been the subject of experimental and theoretical studies by Grannick and coworkers. We find that the bulk Janus systems give rise to surprising equilibrium structure and dynamics which can be tuned through both the volume fraction and the interactions. The coarse-grained model provides surprisingly good agreement with the more detailed particle-model for the equilibrium structure while overestimating the relaxation rates.

<sup>1</sup>This research partially supported by NSF CHE 1112067 utilizing HPC resources provided through NSF CHE 0946869 and XSEDE No. CTS090079.

Rigoberto Hernandez School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA 30332-0400

Date submitted: 29 Nov 2011

Electronic form version 1.4