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Study of the Effect of Ellipsoidal Shape on the Kern and Frenkel Patch Model[1] THIENBAO NGUYEN, JAMES GUNTON, JEFFREY RICKMAN, Lehigh University — In their work on the self-assembly of complex structures, Glotzer and Solomon (Nature Materials 6, 557 - 562 (2007)) identified both interaction and shape anisotropy as two of several means to build complex structures. Advances in fabricating materials and new insights into protein biology have revealed the importance of these types of interactions. The Kern and Frenkel (J. Chem. Phys. 118, 9882 (2003)) model of hard spheres carrying interaction patches of various sizes has been used extensively to describe interaction anisotropies important in protein phase transitions. However their model did not also account for shape anisotropy. We studied the role of both shape and interaction anisotropy by applying N=2 and N=4 attractive Kern and Frenkel patches with an interaction range to hard ellipsoids with various aspect ratios and patch coverages. Following Kern and Frenkel, we studied the liquid-liquid phase separation of our particles using a Monte Carlo simulation. We found the critical temperatures for our model using the approximate law of rectilinear diameter and compared them with the original results of Kern and Frenkel. We found that the critical temperatures increased both with aspect ratio and percent coverage.

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