Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Self-assembly of anisotropic colloidal particles under confinement
CARLOS AVENDANO JIMENEZ, FERNANDO ESCOBEDO, Cornell University
— We perform molecular simulations of two novel anisotropic colloidal particles under confinement. The first is an ensemble of hard-hemispheres (mimicking mushroom cap colloids [1]) confined between two parallel walls separated by a distance H. We simulated: a) Low values of H that restrict the rotation of the particles (in a monolayer) where three main dense crystal structures are found: buckled phase, square, and triangular structures. (b) Large values of H where the particles are able to fully rotate; here parallel (spheres-like) or anti-parallel (column-like) dimers are observed which form ordered structures with triangular and rectangular symmetries at high densities. The second system is a model of hard-square particles with rounded corners. Recently, Zhao et. al. have reported the phase behaviour of monolayers of polymeric squares platelets with rounded corners, assembled at the bottom of the container [2]. This system exhibits the formation of a hexagonal rotator phase and the rhombic crystal phase that were not observed in earlier simulations of squares [3] which found instead a tetratic and square crystal phases. By interpolating between hard discs and hard squares, we map out the phase diagram as a function of the roundness of the particles and resolve the discrepancies of the earlier studies. [1] Riley and Liddell, Langmuir 26, 11648 (2010). [2] Zhao, Bruinsma, and Mason, PNAS 108, 2684 (2011). [3] Wojciechowski and Frenkel, Comp. Met. Sci. Technol. 10, 235 (2004).

Fernando Escobedo
Cornell University

Date submitted: 29 Nov 2011 Electronic form version 1.4