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DENSITY FUNCTIONAL THEORY OF HARD COLLOIDAL PARTICLES: FROM BULK TO INTERFACES



Shaker Verlag Mai 2013, 2013. Buch. Book Condition: Neu. 24x17x cm. Neuware - In this work about density functional theory of hard colloidal particles, spheres, spherocylinders, and dumbbells are investigated in the bulk and at interfaces. Therefore, the theoretical framework of density functional theory (DFT) and fundamental measure theory (FMT) is introduced first. Then, FMT functionals are applied to hard-sphere systems to obtain free energies and density distributions for the (fcc) crystal and the fluid phase. The free energies are...

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