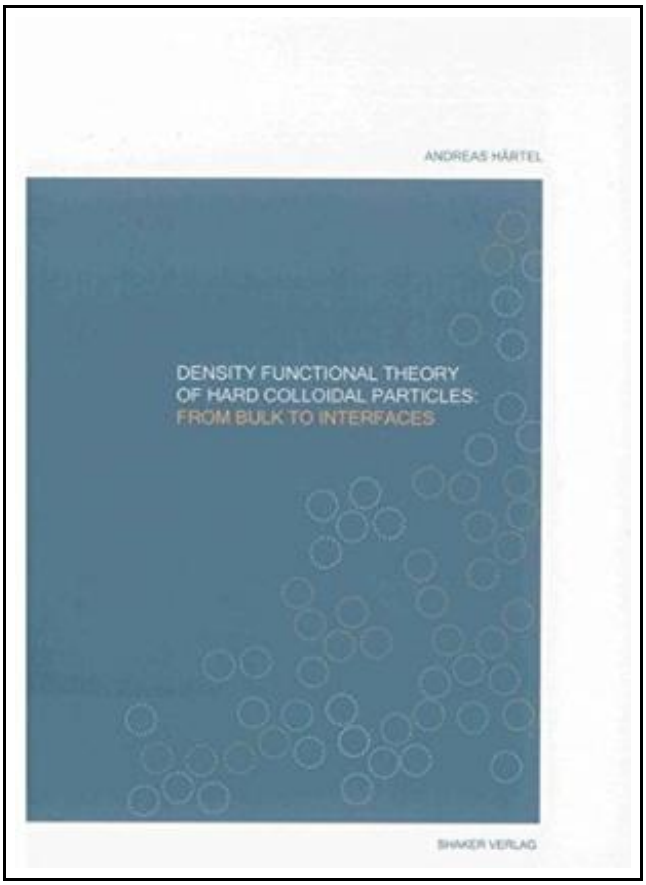
Density functional theory of hard colloidal particles: From bulk to interfaces



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Reviews

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

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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 in good agreement with Monte Carlo (MC) simulation results, which is also reflected in the density distributions around single lattice sites. From the studied variants of FMT only the White Bear mark II (WBII) functional shows qualitatively correct behavior, which implies that only the WBII functional is a promising candidate for further studies of problems involving crystallization. Accordingly, accurate values for the anisotropic hard-sphere crystal-fluid surface tensions and stiffnesses have been predicted by using the WBII approach in combination with MC simulations. Quantitative agreement between FMT and simulations is found, where FMT predicts a tension of 0.66 kBT/s 2 with a small anisotropy of about 0.025 kBT. The corresponding stiffnesses are determined with e.g. 0.53 kBT/s 2 for the (001) orientation and 1.03 kBT/s 2 for the (111) orientation of the interface, where kBT is the thermal energy and s is the diameter of the hard spheres. However, the anisotropy in the tension is crucial for the transformation to stiffnesses, which differ up to a factor of 4. Moreover, the results from theory and simulation are compared with existing experimental findings and classical nucleation theory is discussed in the context of analyzing experimental results. In another sense, FMT has also been applied to non-spherical particles. For this purpose, the recently developed extended deconvolution FMT (edFMT) has been applied to systems...

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