# Computer Simulations of Self-Assembled Mesocrystals formed by Iron Oxide Nanocubes

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Monte Carlo simulations of the packing and thermodynamic properties of iron oxide nanoparticles in the shape of truncated cubes have been performed. Attractive Van-der-Waals interaction in Hamaker approximation and dipolar interaction between particles were considered. A parallel Monte-Carlo algorithm for modeling of self-assembly of nanoparticles was implemented in the computer program. The algorithm include anisotropic simulation shell fluctuations treated within Wang-Landau entropic sampling approach, as well as realistically described interaction between the nanoparticles taking into account their shapes.