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Density functional theory simulations of ferrihydrite nanoparticle aggregation via organic surface complexation

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Aggregation of soil particles is critical for soil health and stability. Studies have demonstrated that organic matter with multiple carboxylate functional groups can lead to aggregation and help preserve organic matter from biodegradation. This study uses density functional theory (DFT) simulations to assess the molecular mechanism and energetics responsible for this phenomenon. We have used periodic DFT calculations in the Vienna Ab-initio Simulation Package (VASP) to model the linkage between two Fe13 nanoparticles and the effect that citrate has on the interparticle distance. The Fe13 nanoparticles with the ferrihydrite structure as published in Michel et al. were solvated with explicit H_2O molecules and modeled with citrate bonded to both particles and free from both particles. The aggregated form decreases the interparticle distance significantly and dramatically lowers the energy of the system. This work has implications for understanding and managing soil aggregation and soil organic matter preservation.