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Molecules coating magnetic nanoparticles for oil-field applications[1] SEBASTIAN ZULUAGA, PRIYANKA MANCHANDA, SOKRATES PANTELIDES, Vanderbilt University — Magnetic nanoparticles have recently attracted significant attention in scientific and industrial communities due to their use in the fields of catalysis, spintronics, biomedical applications, and oil recovery and reservoir characterization. However, these nanoparticles have to be protected with a coating layer of molecules that prevents the nanoparticles from oxidation, which is known to occur in air, and from agglomeration into larger nanoparticles. Therefore, the binding of the molecules to the nanoparticles is critical before a large scale implementation can be done. Here we report results of density functional theory calculations on several molecules (methylamine, acetic acid, boronic acid, ethyl phosphate, and ethyl trihydroxysilane) and magnetic nanoparticles (Fe_3O_4, $NiFe_2O_4$, and Fe_3C). We focus on two main points: 1) the bond strength between the organic molecule and the nano particle, and 2) how, H_2O and H^+ in the oil well may facilitate the desorption of the molecules. The results show that H^+ and H_2O molecules facilitate the desorption of molecules reducing the bond strength by several eV. On the other hand, the results allow us to identify and design molecules that exhibit the best performance in protecting each nanoparticle.

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Sebastian Zuluaga
Vanderbilt University

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