# CHALLENGES IN THE MODELING OF METAL NANOPARTICLE REACTIVITY

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**Abstract**

The large surface-to-volume ratio of nanoparticles can lead to surprising surface and quantum size effects. The reactivity of nanoparticles is of special interest, however, required highly accurate theoretical description and modeling of the nanoparticle reactivity is still challenging.[1] We discuss computational methods and models that can be applied to study reactions of metal nanoparticles and consider their benefits and limitations. We report current progress in calculations through recent examples treating the reactivity of nano zero-valent iron (nZVI) particles.[2-4] We consider reactivity of iron clusters depending on the cluster size and the local geometrical structure and we compare our recent theoretical results with experimental reaction kinetics.[5]

**Keywords:** Nanoparticles, Modeling, Reactivity, Metals, nZVI

**LITERATURE:**

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