

# Quantum chemical modeling arsenic (III,V) adsorption and oxidation on manganese oxides

## GEOC 40

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Mn(III,IV)-oxides strongly regulate arsenic mobility, toxicity and bioavailability by oxidizing arsenite (As(III)) to arsenate (As(V)) in the natural environment. Here we used quantum chemical calculations to investigate the adsorption and oxidation of arsenic (As(III) and As(V)) on the surface of Mn(III, IV)-oxides. Several possible electron transfer processes were modeled and adsorption affinities between arsenite/arsenate and Mn(III)/Mn(IV) oxides were compared. The results help explain certain arsenite oxidation behavior, such as 1) possible arsenite oxidation pathways, electron transfer or substitution mechanism? 2)inhibition mechanisms of arsenite oxidation by arsenate, and 3) the role of Mn(III) in arsenite oxidation. A better understanding of arsenite oxidation will help predict arsenic fate and transport of arsenic in the environment.

[Biogeochemical Redox Processes in Soils and Sediments](#)

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