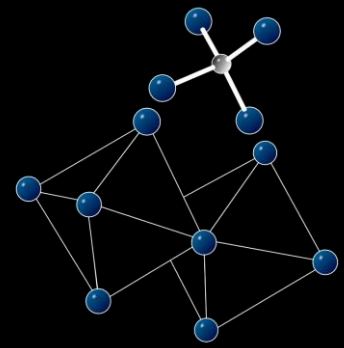
Ion complexation modelling of ferrihydrite:

From fundamentals of metal (hydr)oxide nanoparticles to applications in soil systems



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Utrecht, 6th of April 2023

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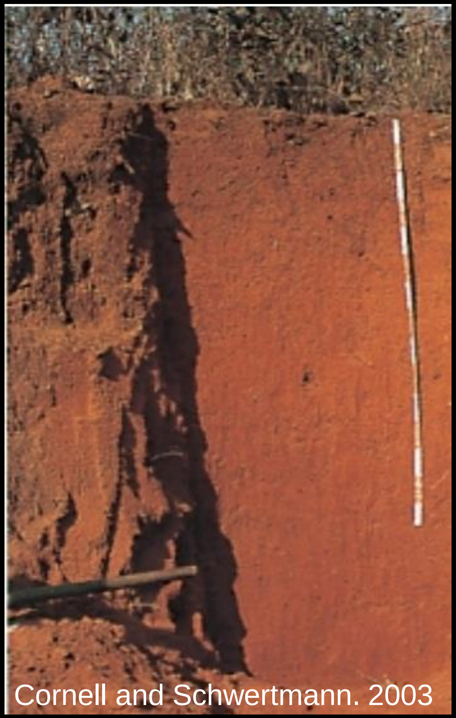
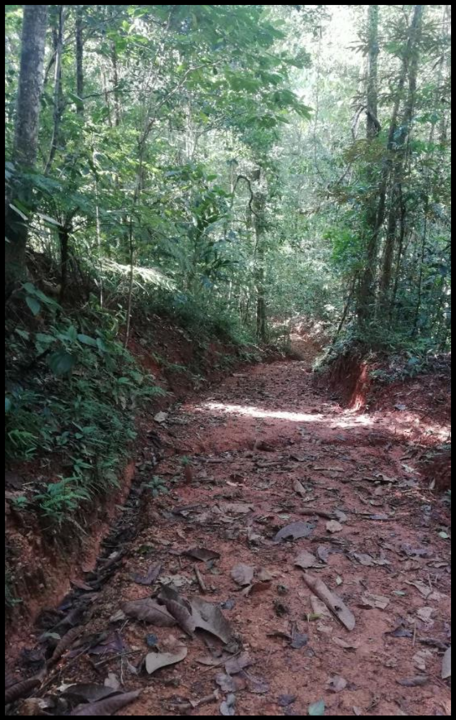
UNIVERSIDAD DE COSTA RICA

WAGENINGEN
UNIVERSITY & RESEARCH

About myself…

- B.Sc. in Agriculture Engineering (University of Costa Rica)
- M.Sc. in Environmental Sciences (Wageningen University)
- PhD in Soil Chemistry and Environmental Geochemistry (Wageningen University)
- Researcher at the Faculty of Agri-Food Sciences and at the Agronomical Research Centre (CIA-UCR)



Metal oxides in soils

- Reactive charged surfaces
- Control availability of nutrients and pollutants
- Soil organic carbon storage

Ferrihydrite nanoparticles

- Most important iron oxide nanoparticle in nature

- Small size (~2–6 nm) → high surface reactivity

  ~1 m^2 soil → 10 million m^2 surface reactivity

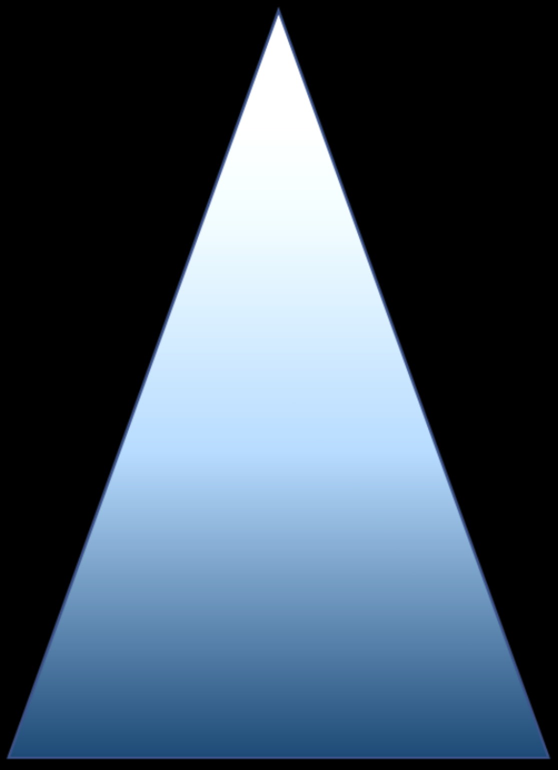
- High affinity for nutrients, pollutants and SOM

Objectives and scope

I. Surface reactivity of ferrihydrite

II. Adsorption of phosphate to ferrihydrite

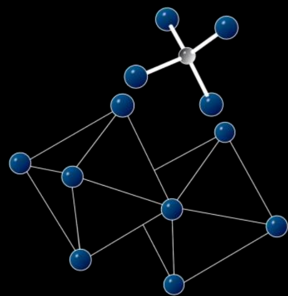
III. Reactivity of natural oxides in soils



I. Reactivity of ferrihydrite

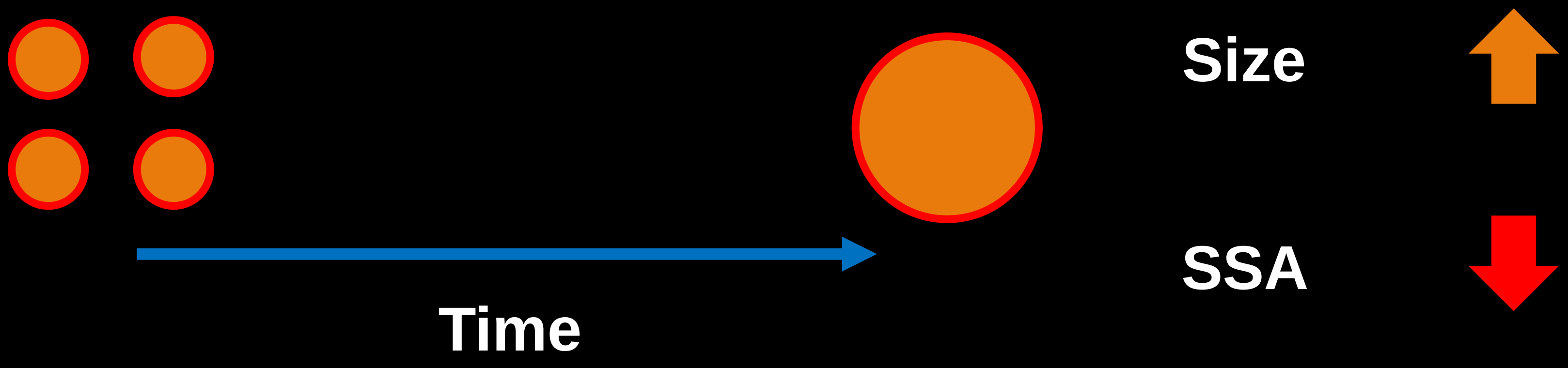
From:

- Mendez J.C., Hiemstra T. 2020. *Chemical Geology.* 532: 119304
- Hiemstra T., Mendez J.C., Li J. 2019. *Environ. Sci. Nano.* 6(3): 820-833

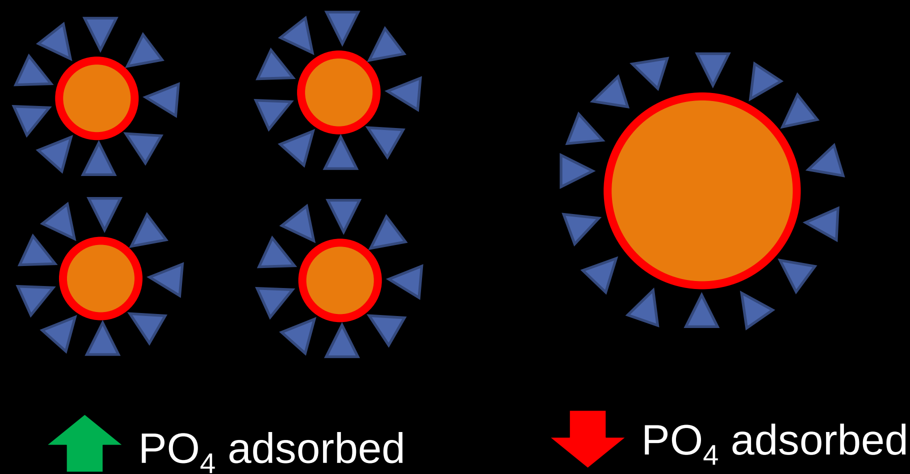


Specific surface area (SSA)

- Defines the **reactivity** of ferrihydrite
- Depends on the formation conditions (e.g. pH)



How to measure the SSA?



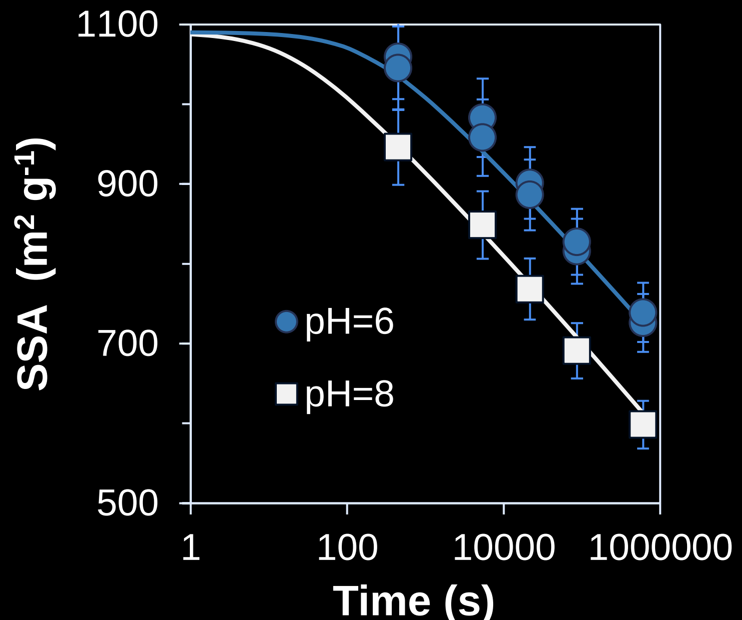
Phosphate as probe molecule

Practical and reproducible

How does the SSA change?

Time and pH dependency of SSA

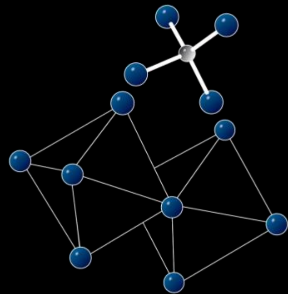
Consistency between ion adsorption experiments



II. Adsorption interactions of phosphate

From:

- Mendez J.C., Hiemstra T. 2020. *Geochim. Cosmochim. Acta.* 286: 289-305
- Mendez J.C., Hiemstra T. 2020. *ACS Earth Space Chem.* 4(4): 545-557
- Mendez J.C., Hiemstra T. 2019. *ACS Earth Space Chem*. 3(1): 129-141



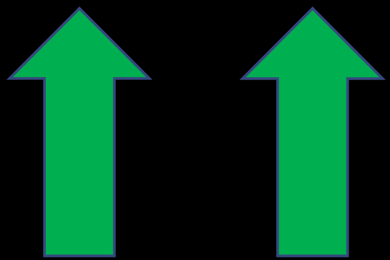
Cooperative adsorption

Cation (**+**) & Anion (**–**)

Competitive adsorption

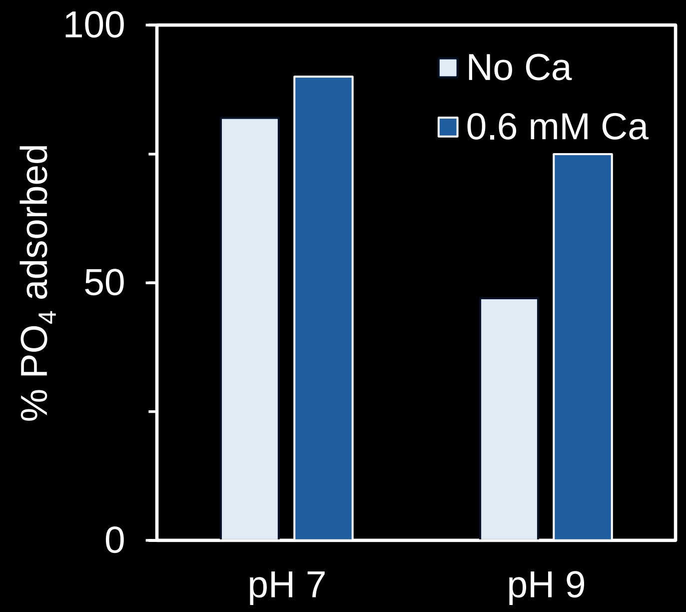
Anion (–) & Anion (–)

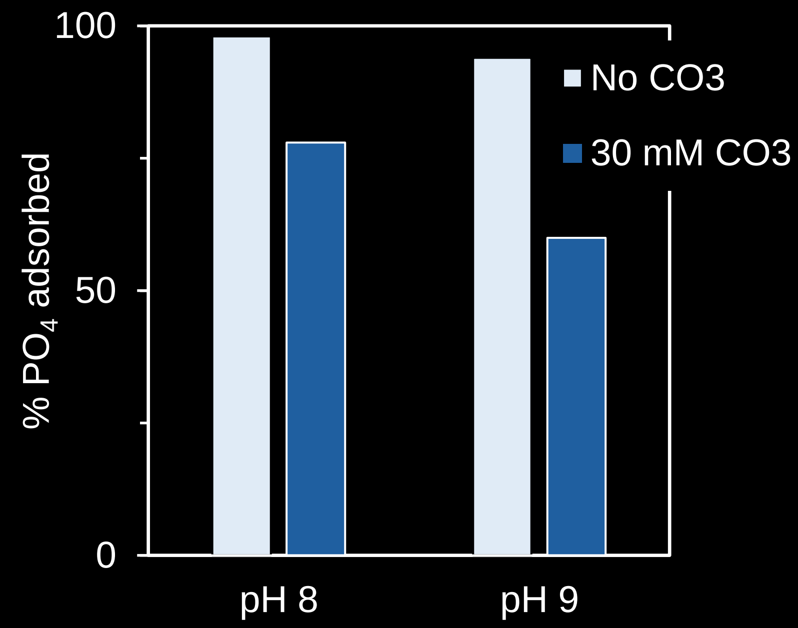
Cooperative adsorption



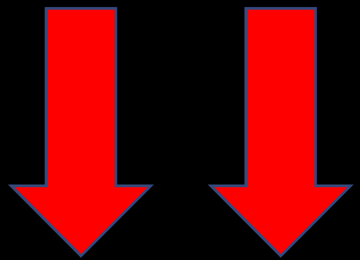
Cation (**+**) & Anion (**–**)

Calcium - Phosphate



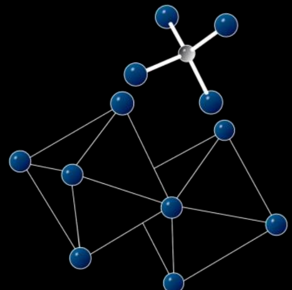


Competitive adsorption



Anion (–) & Anion (–)

Carbonate - Phosphate



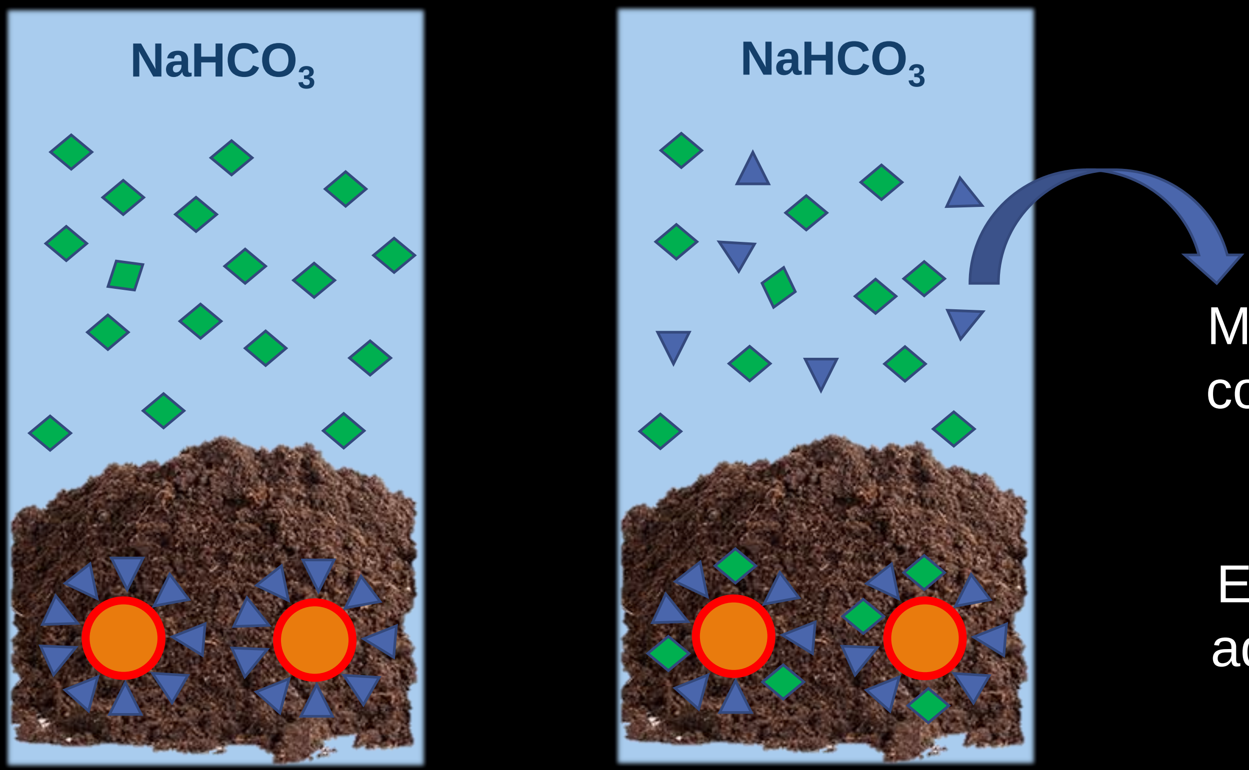
III. Applications to soil samples

From:

- Mendez J.C., Koopmans G.F., Hiemstra T. *Environ. Sci.Technol. 54: 11990 - 12000*
- Mendez J.C.[*], Van Eynde E.[*], Hiemstra T., Comans R.N.J. *Geoderma.* 406:115517
- Van Eynde E.[*], Mendez J.C., Hiemstra T., Comans R.N.J (*to be submitted*)

Ferrihydrite as proxy for natural oxides

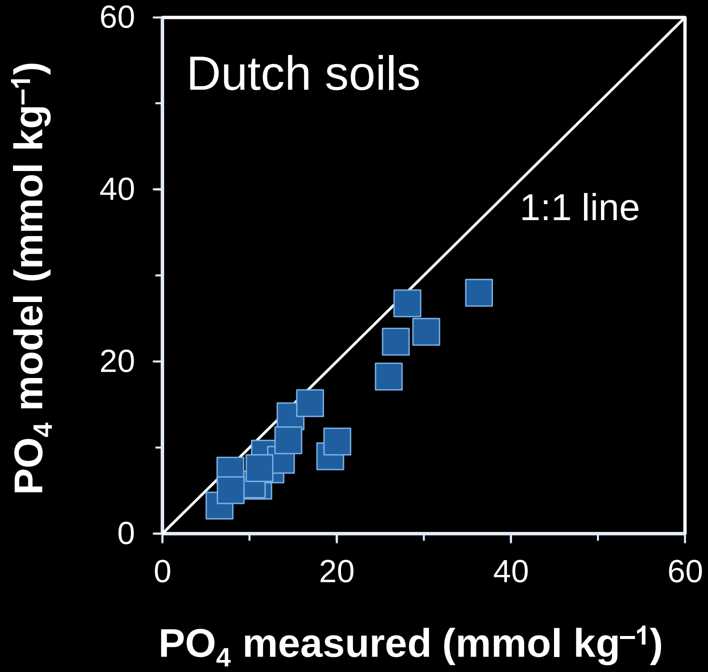
- Interpretation of PO_4 – CO_3 in soil extractions

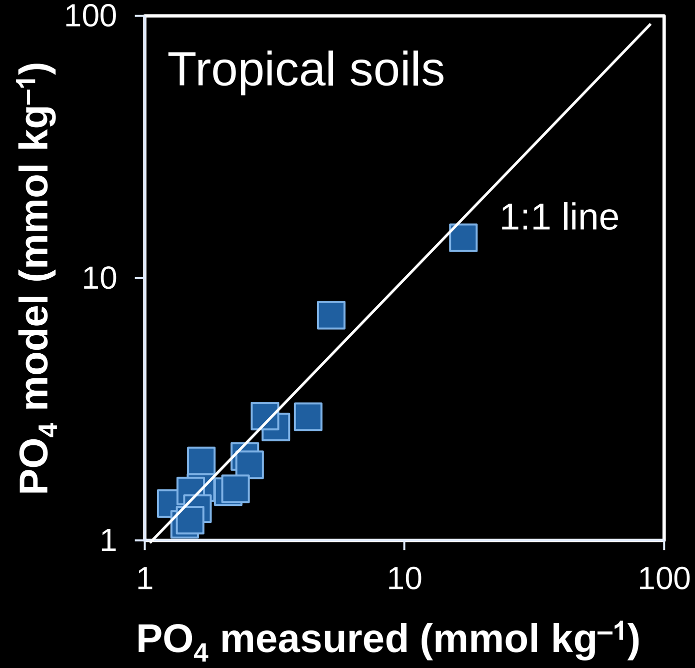


Measure PO_4 concentration

Estimate total adsorbed PO_4

Ferrihydrite as proxy for natural oxides





- “Ferrihydrite-like” nanoparticles (~2–5 nm) control the surface reactivity in these soils

Implications

- Better understanding and predictions of the availability of nutrients and pollutants
- Role of metal (hydr)oxides in soil organic carbon stabilization

Summing up

- Improved insights into surface reactivity of ferrihydrite

- Understand the role of ferrihydrite in the reactivity of soils

- Interactions affecting PO_4 availability in soils

Applications in my current research

Reactivity of nanocrystalline minerals in volcanic soils

- Abundance of highly reactive nanocrystalline minerals
- Low content of available P and high P retention capacity
- Low efficiency of P fertilizer applications

Thank you!

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