

Disproportionation in gas-phase di- manganese oxide cluster revealed by X- ray absorption spectroscopy

Olesya Ablyasova
PhD student

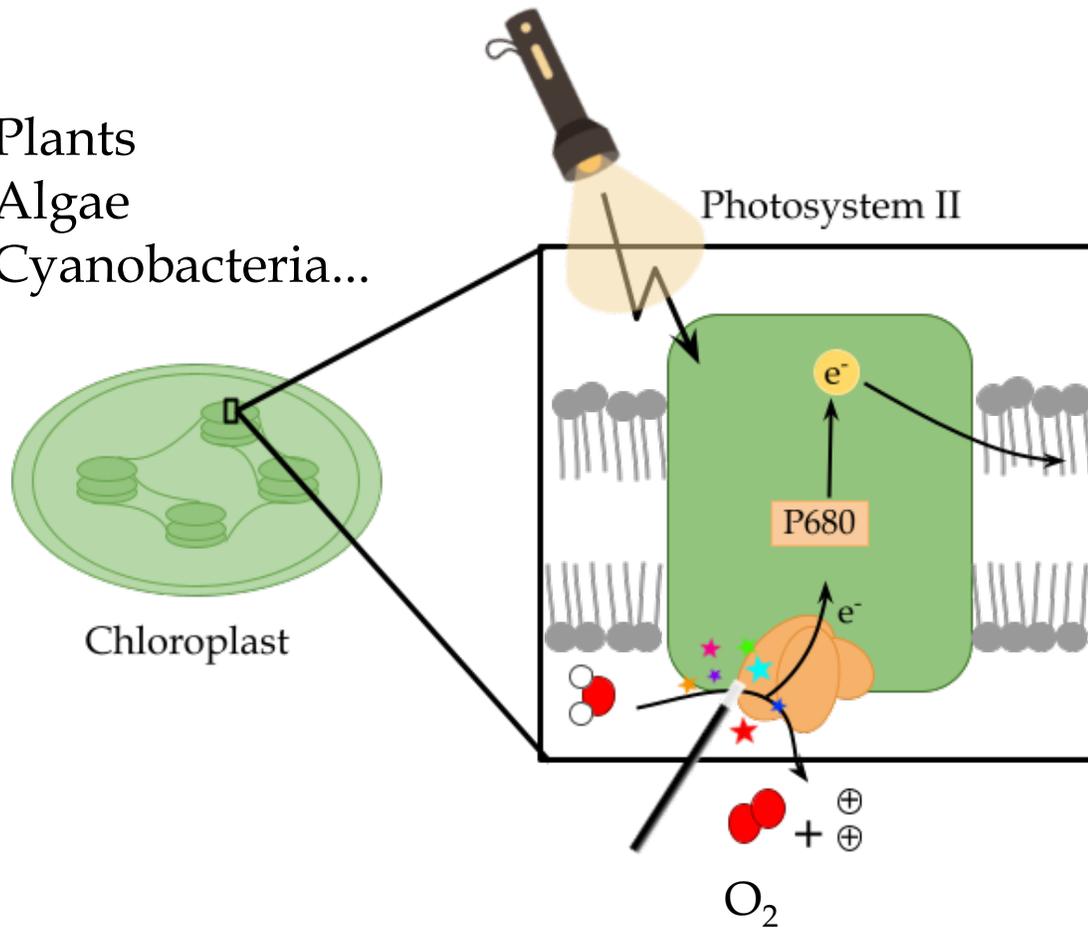
See poster
Aryna Hreben

26.11.2022 Karlsruhe
The German Conference of Women in Physics 2022

Photosystem II from Chloroplasts

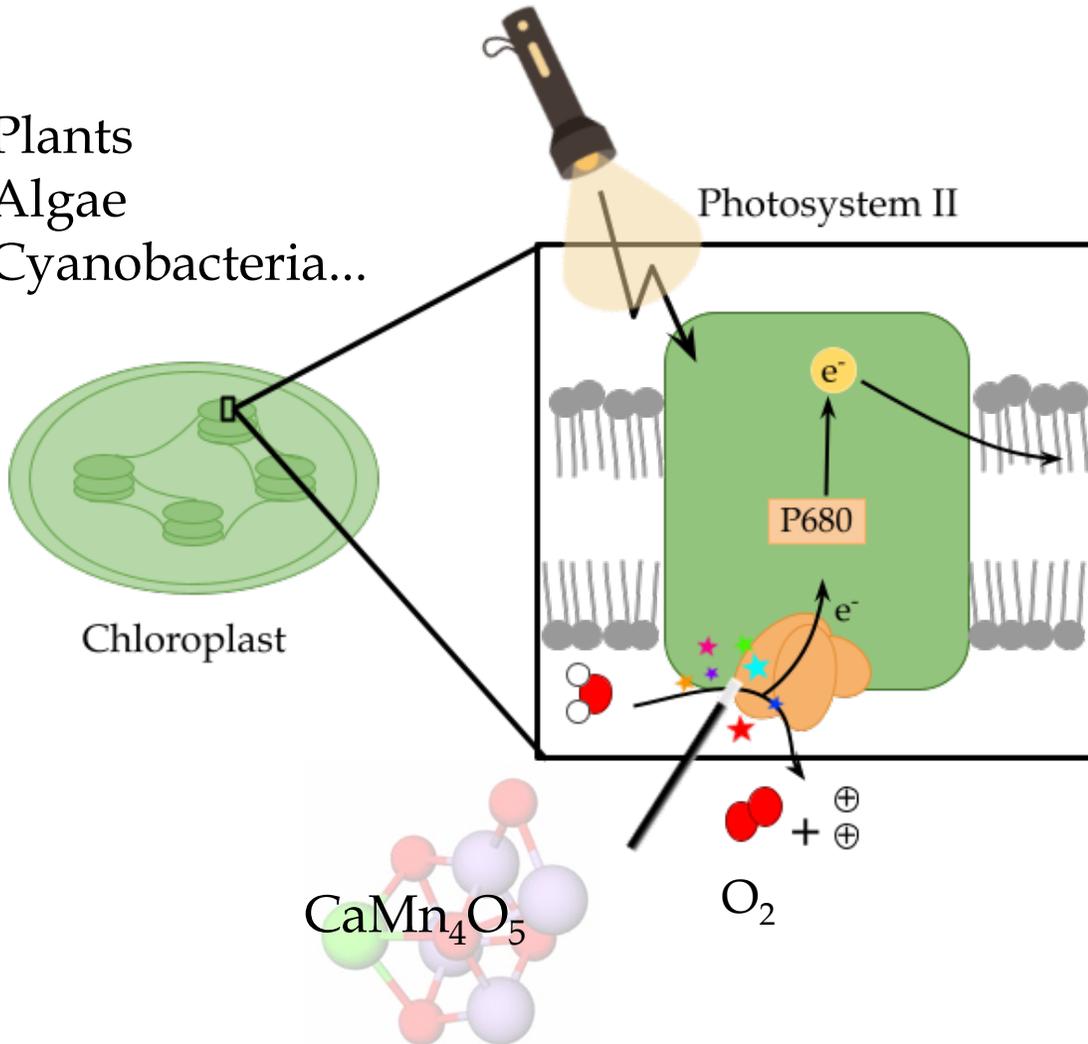


Plants
Algae
Cyanobacteria...



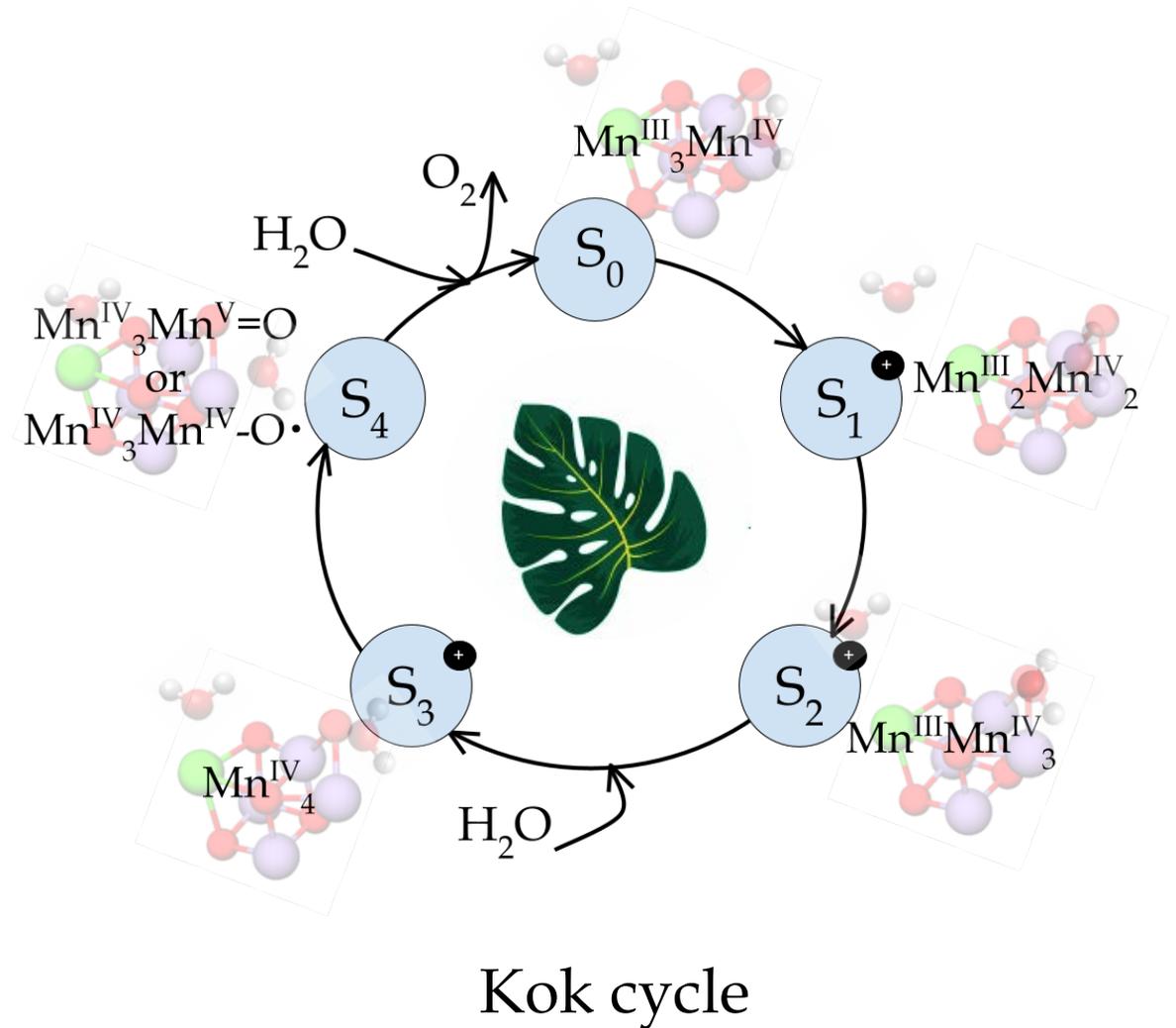
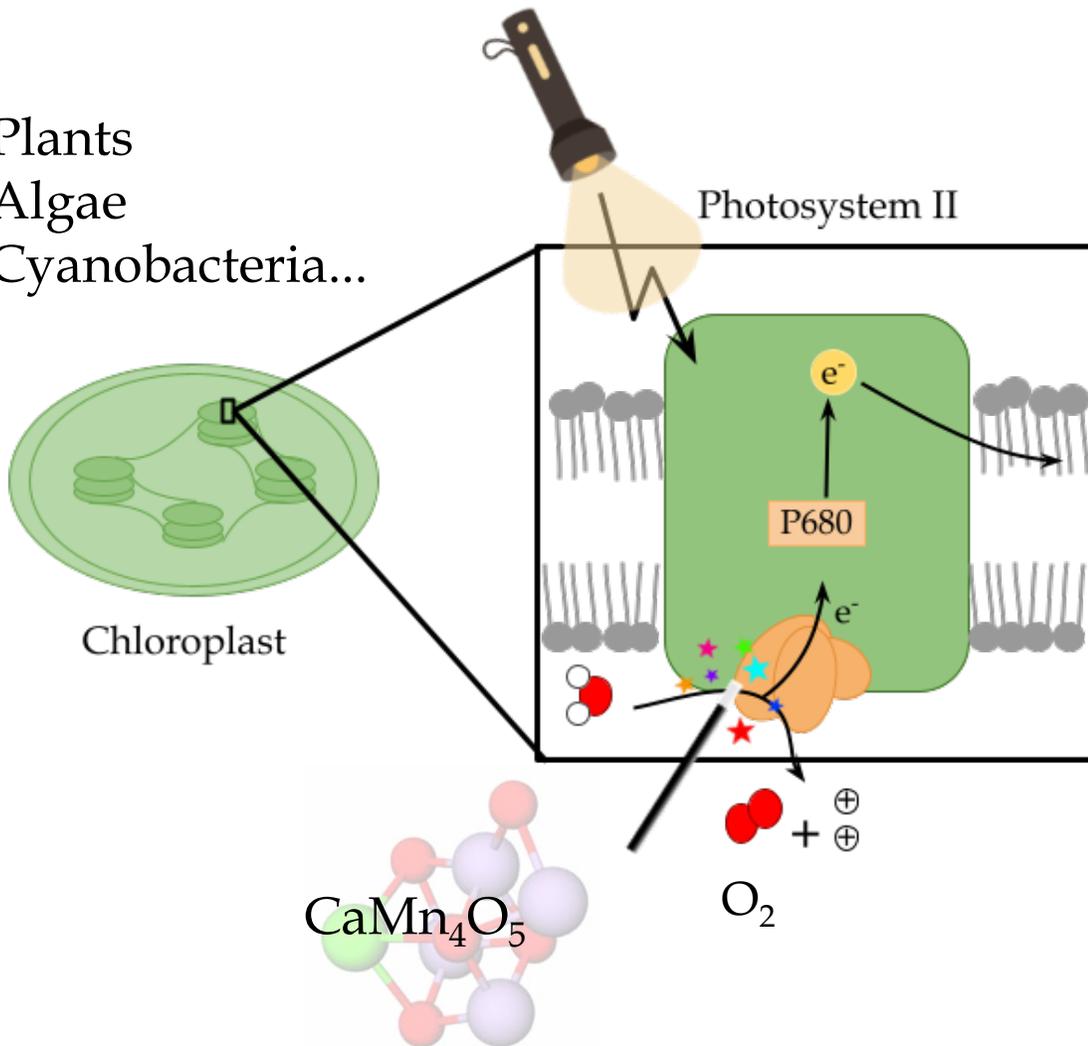
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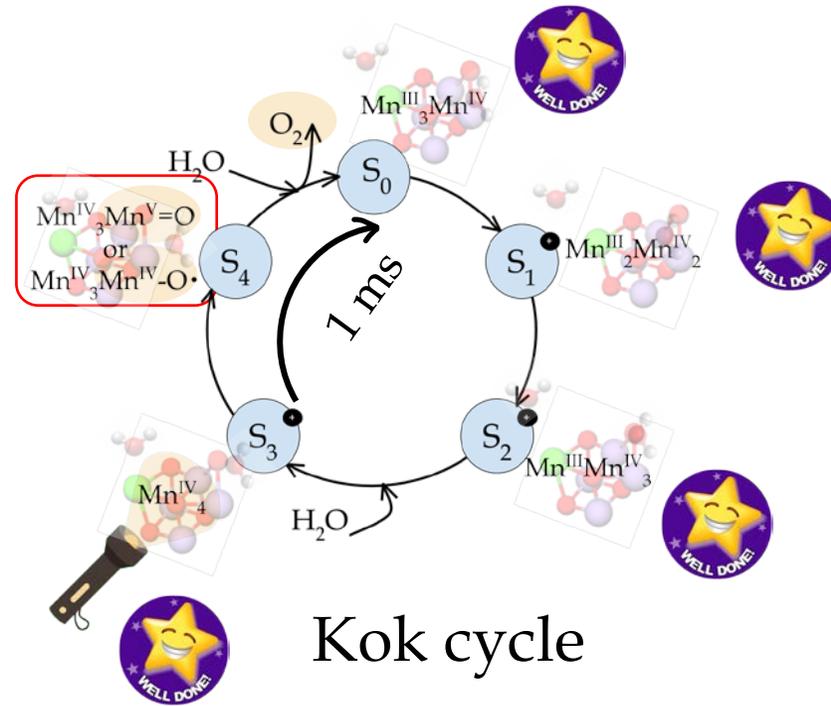


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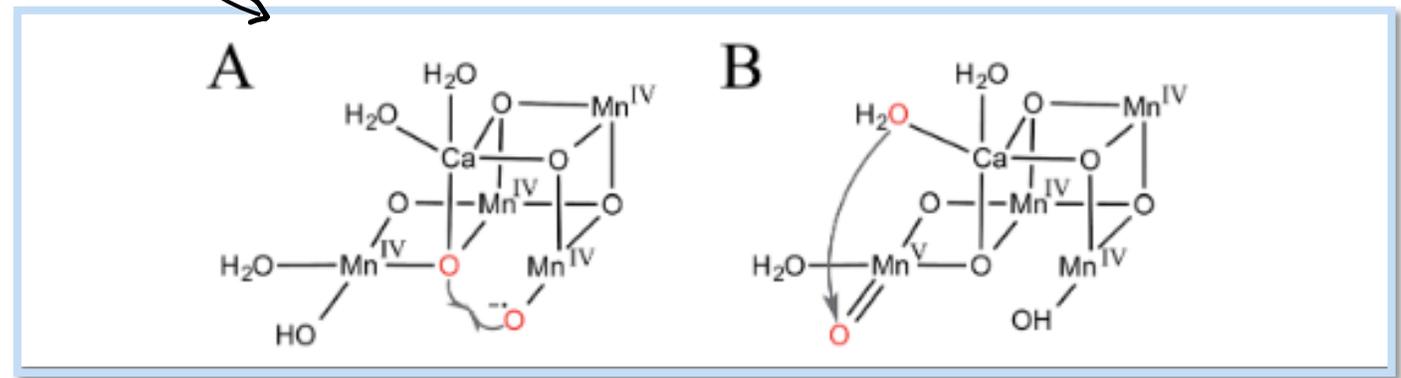
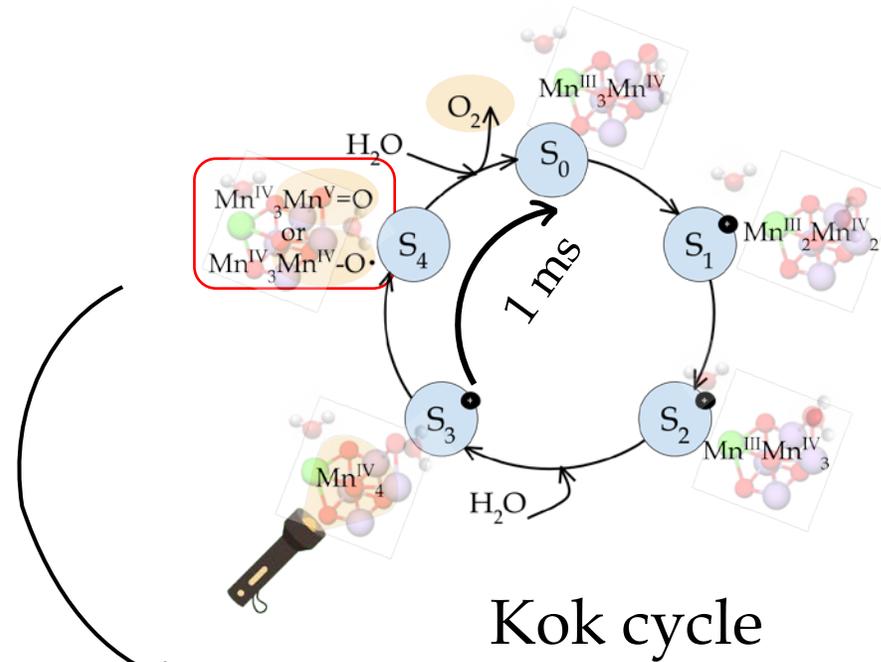
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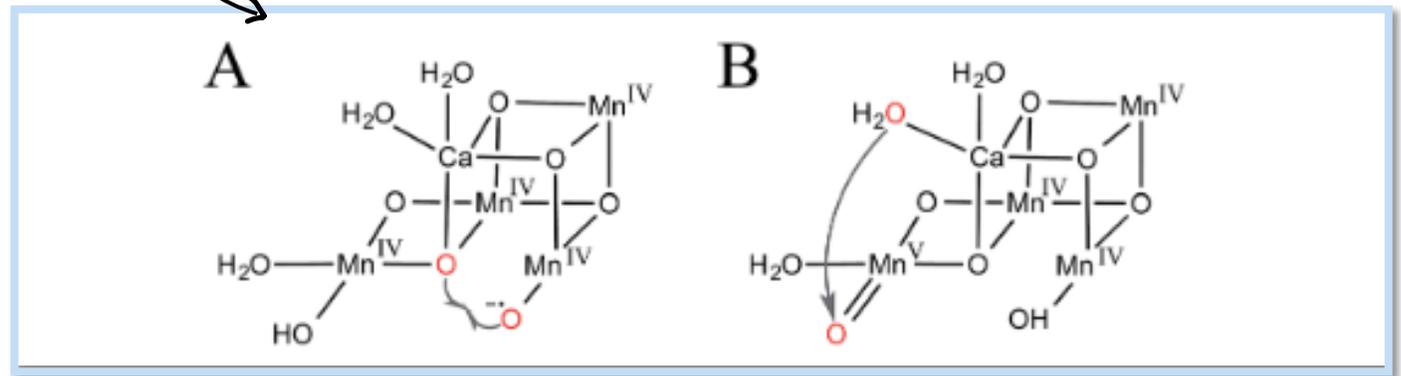
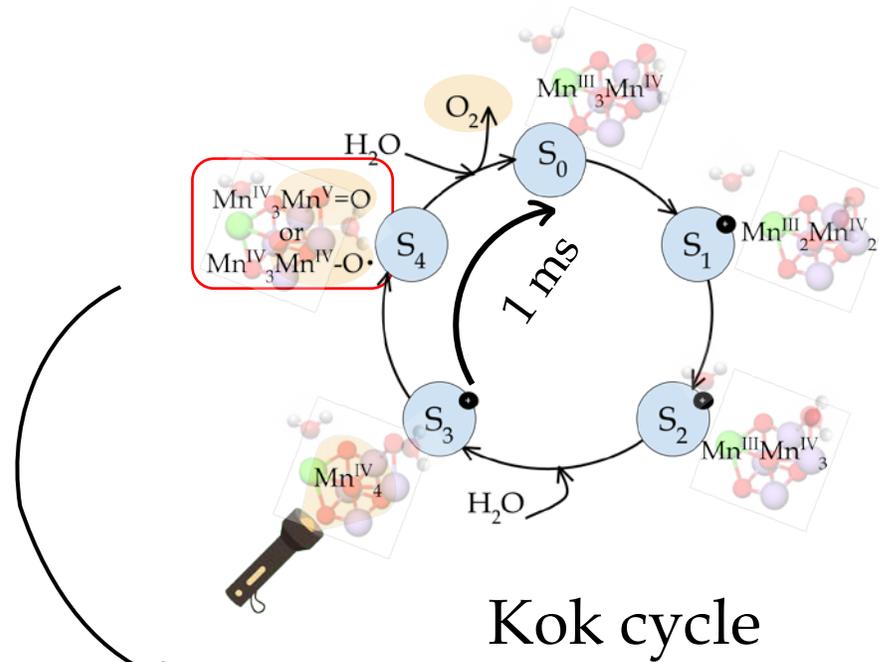
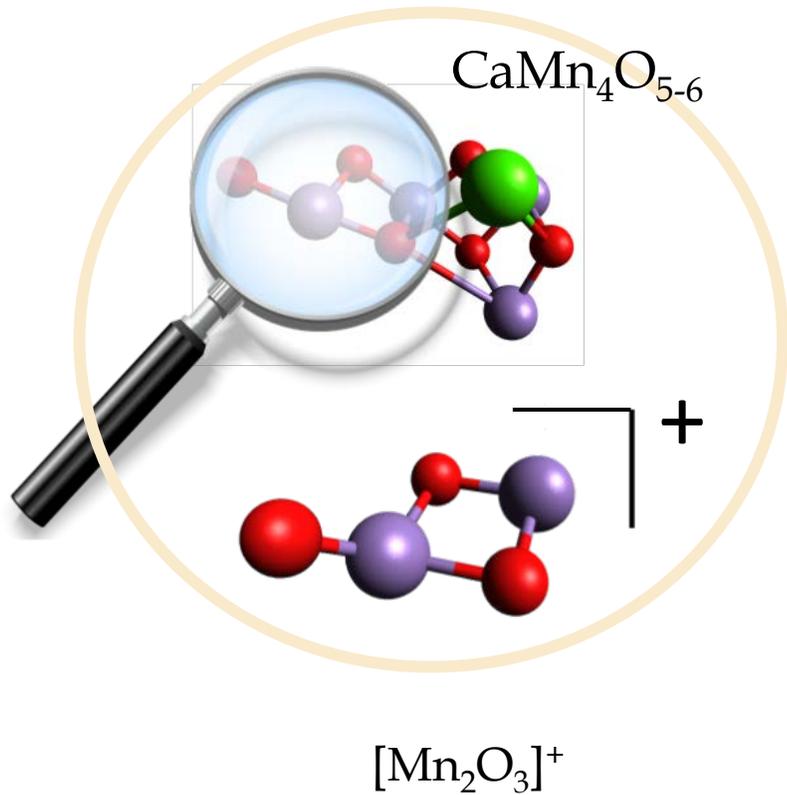


Kok cycle



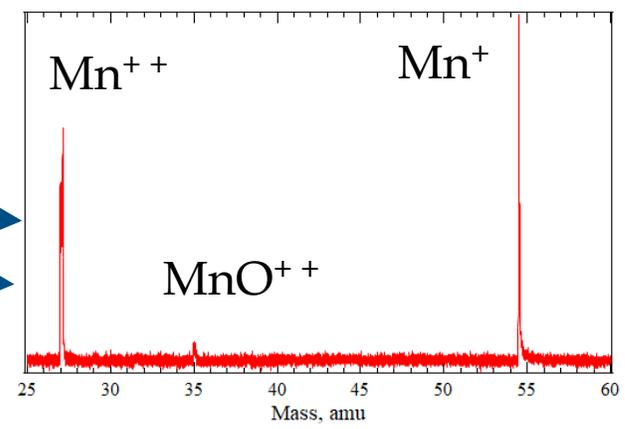
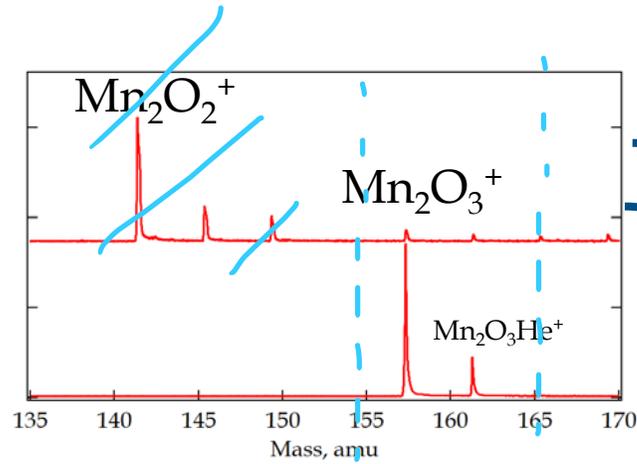
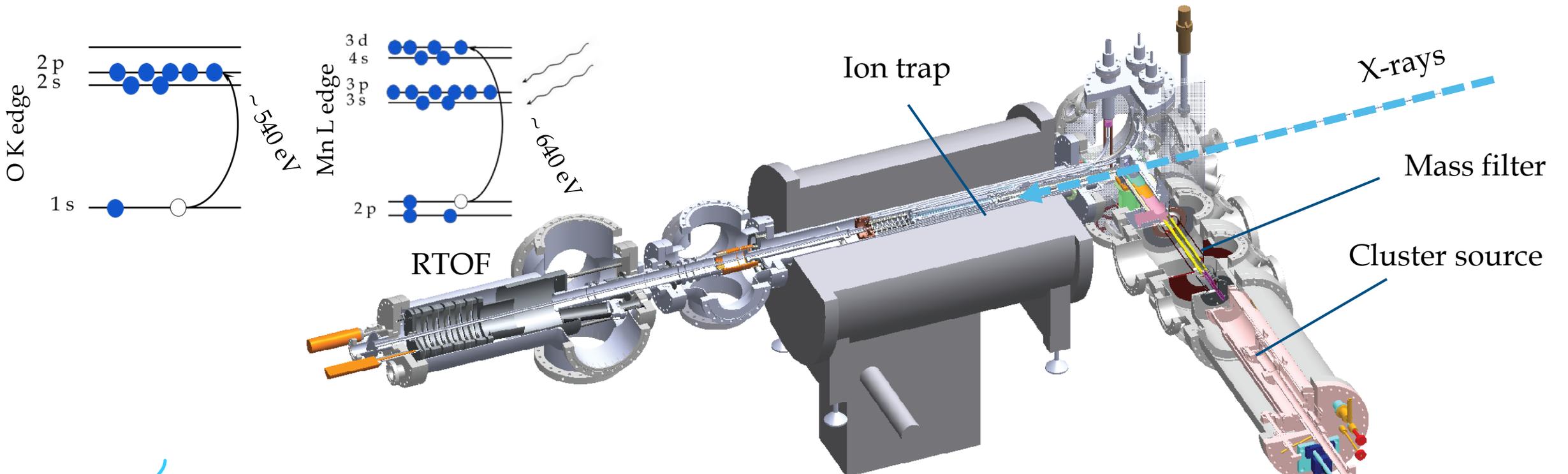
Faraday Discuss., 2015,185, 37-50

Photosystem II from Chloroplasts

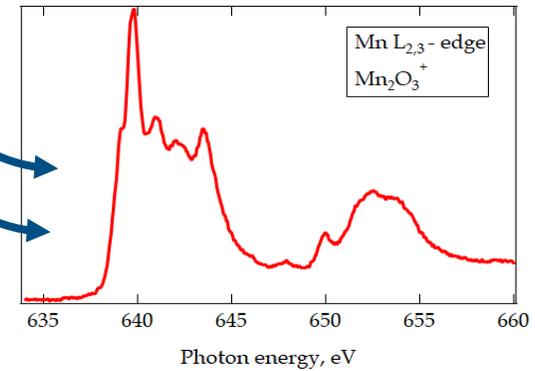
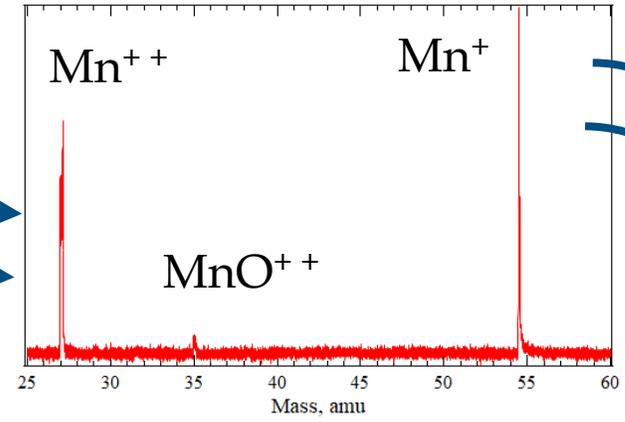
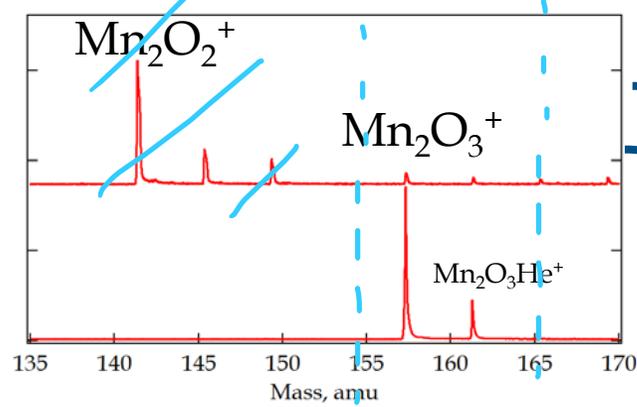
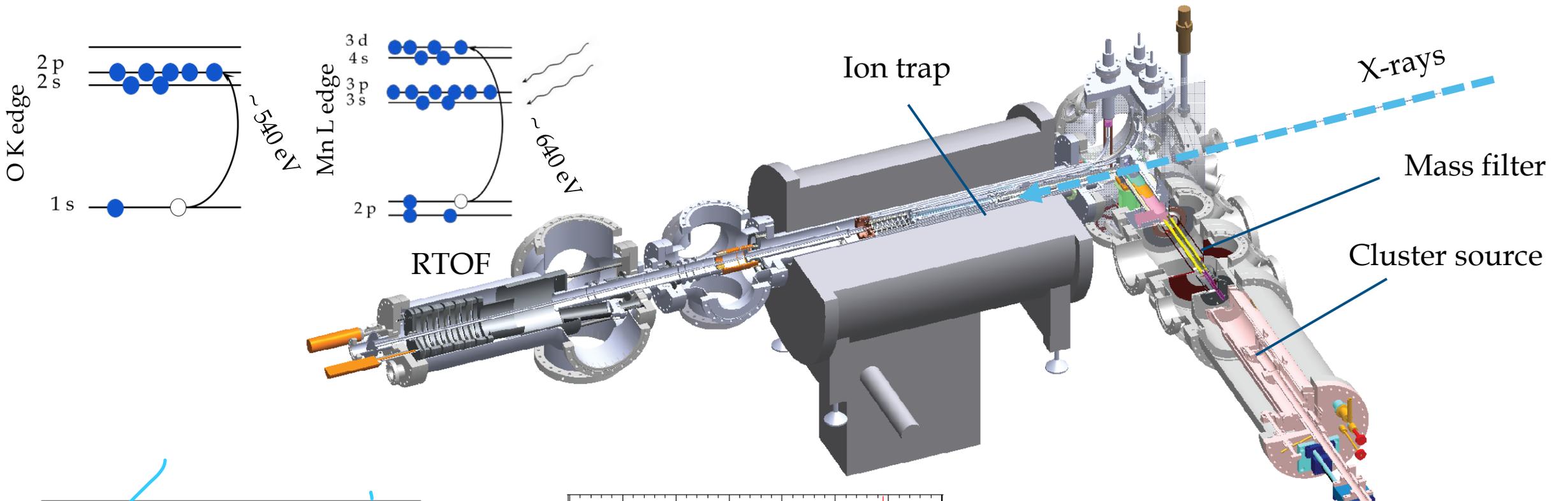


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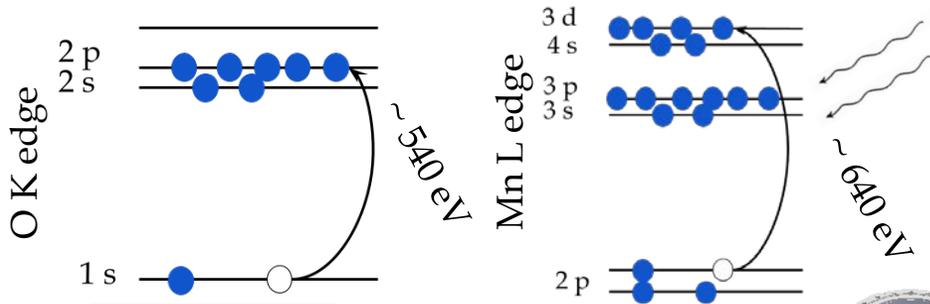
Ion Trap Setup



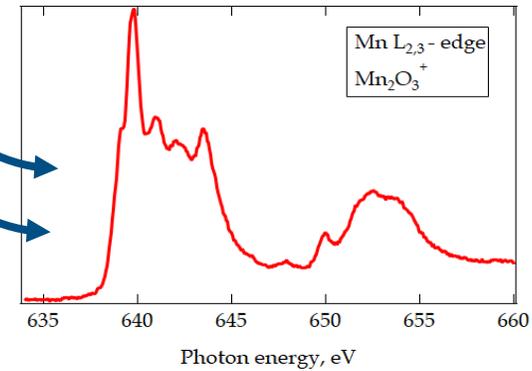
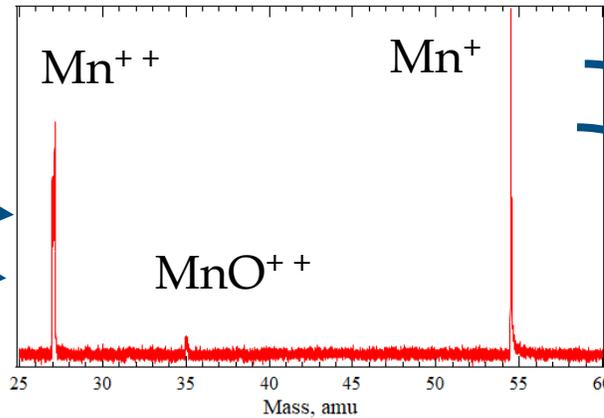
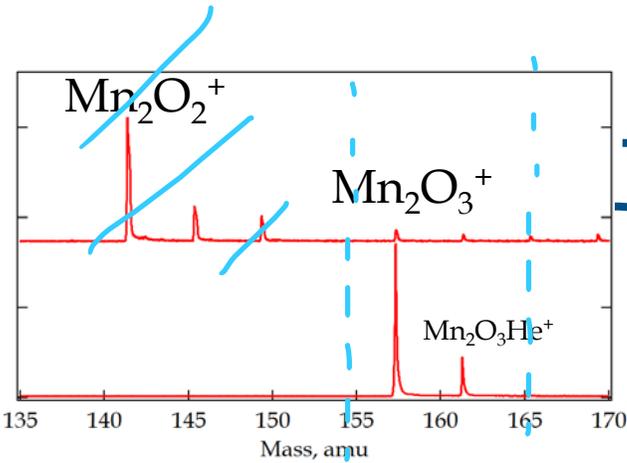
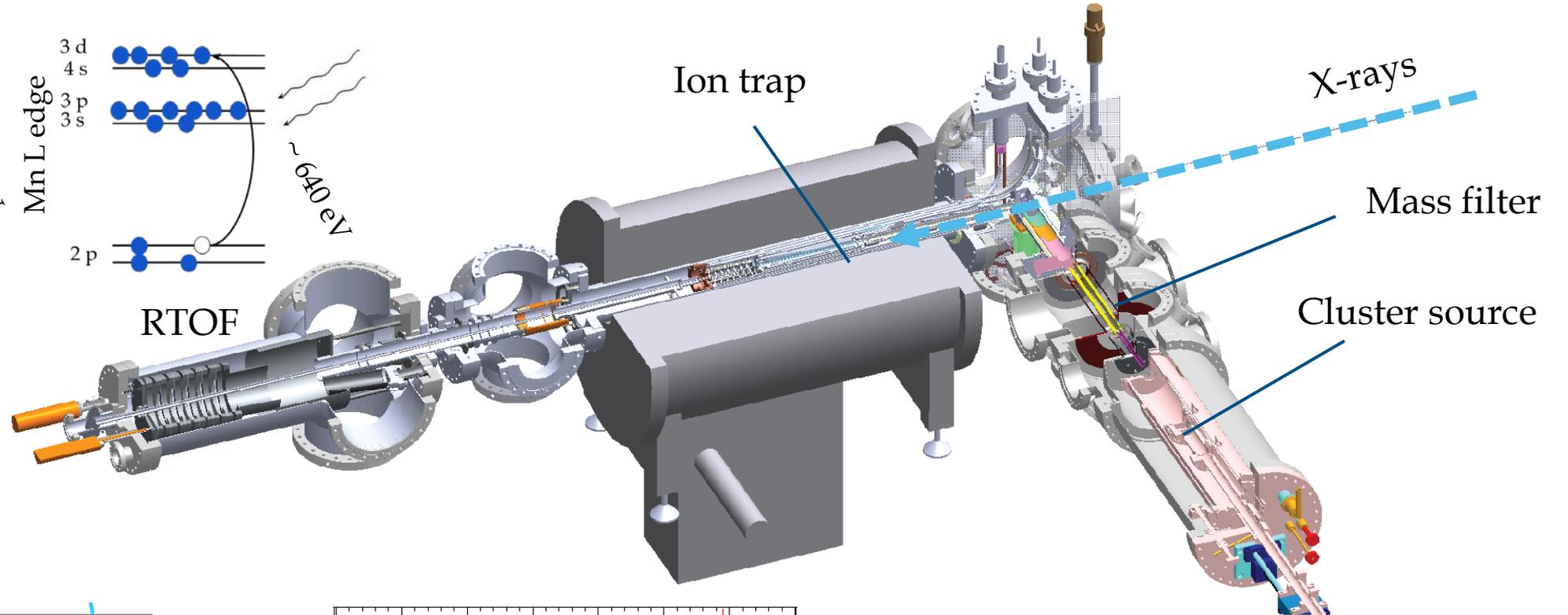
Ion Trap Setup



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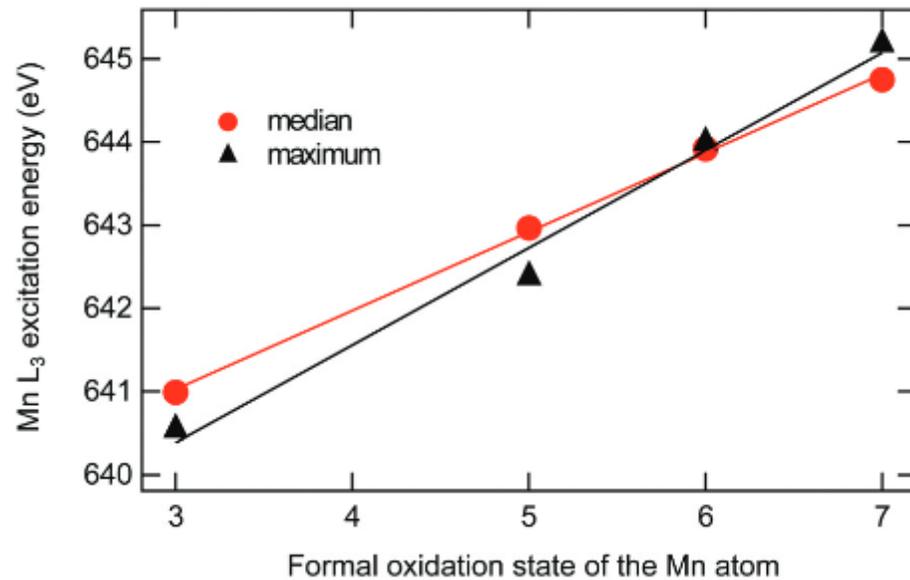


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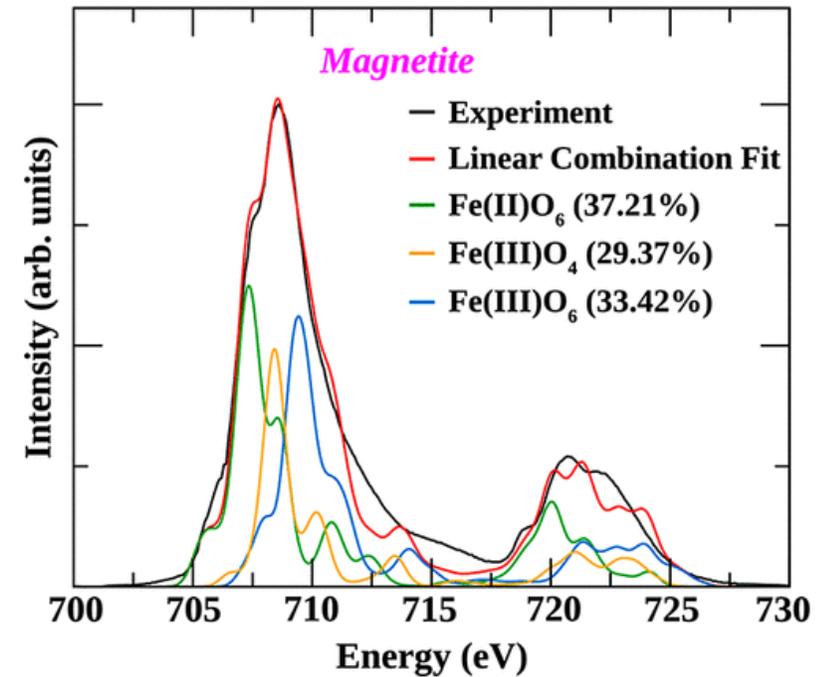


Lessons from the 3d metal oxides:

①



②



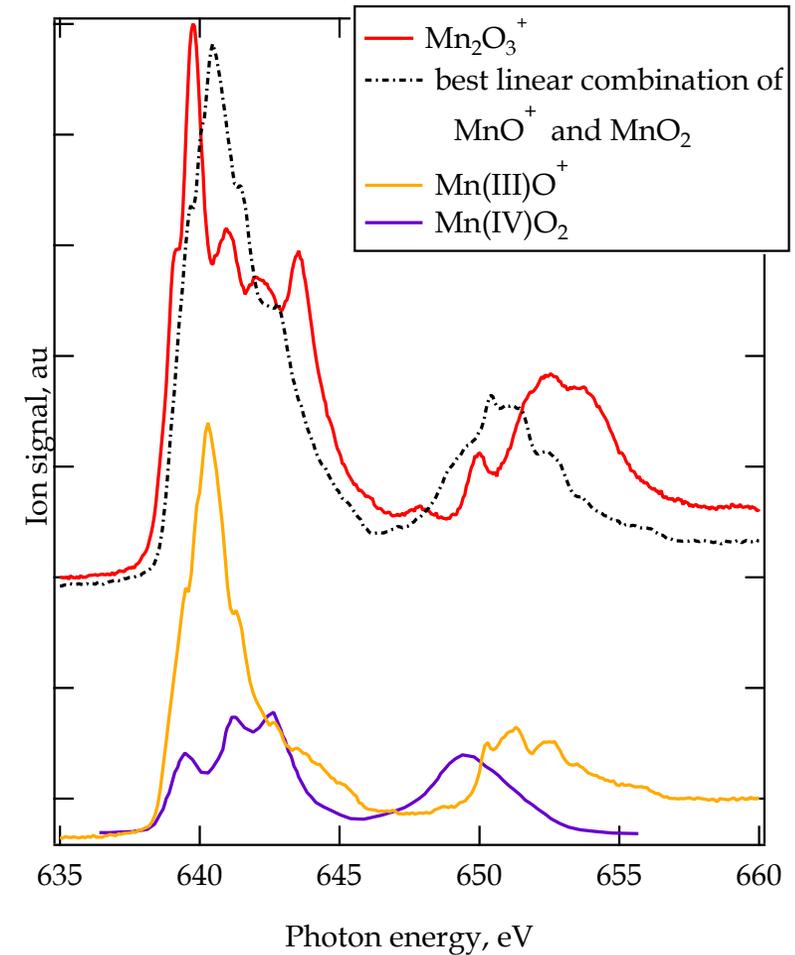
Phys. Chem. Chem. Phys., 2022, 24, 3598-3610

J. Phys. Chem. A 2017, 121, 40, 7613–7618

O. Ablyasova, HZB

Mn L edge

$$\text{Cos Sim} = \frac{A * B}{\|A\| * \|B\|}$$

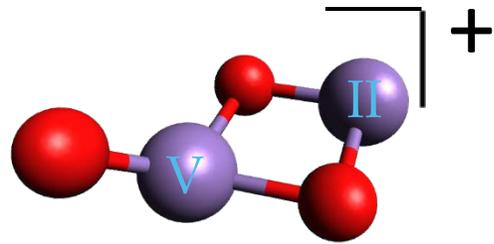


Cosine similarity 0.9454

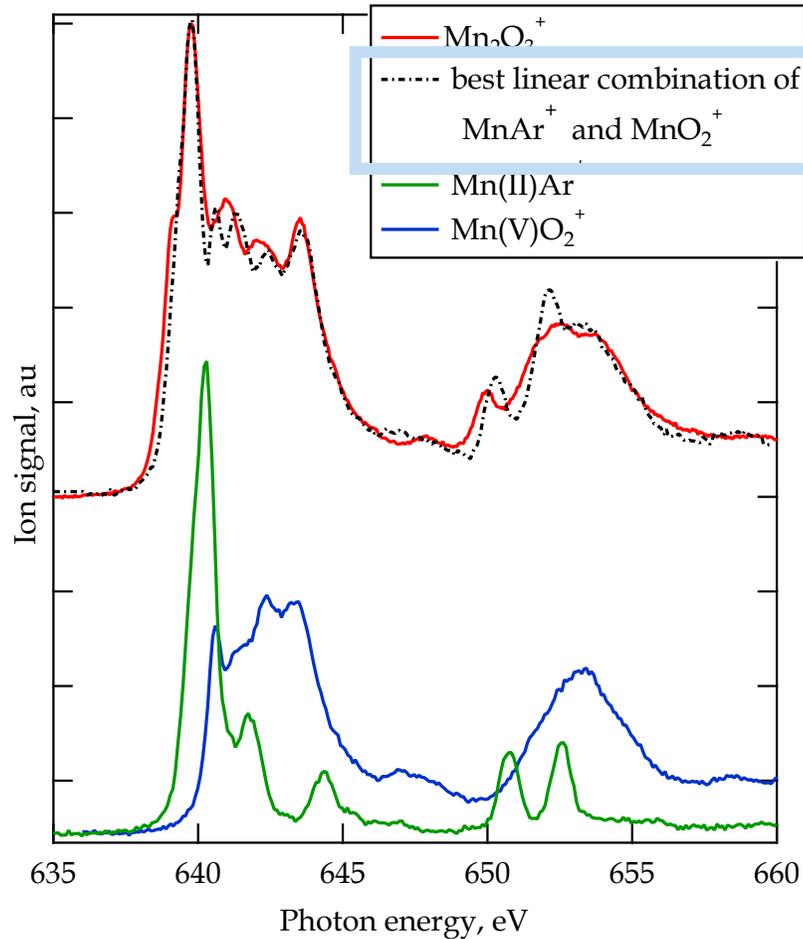
Experimental determination of oxidation state

Mn L edge

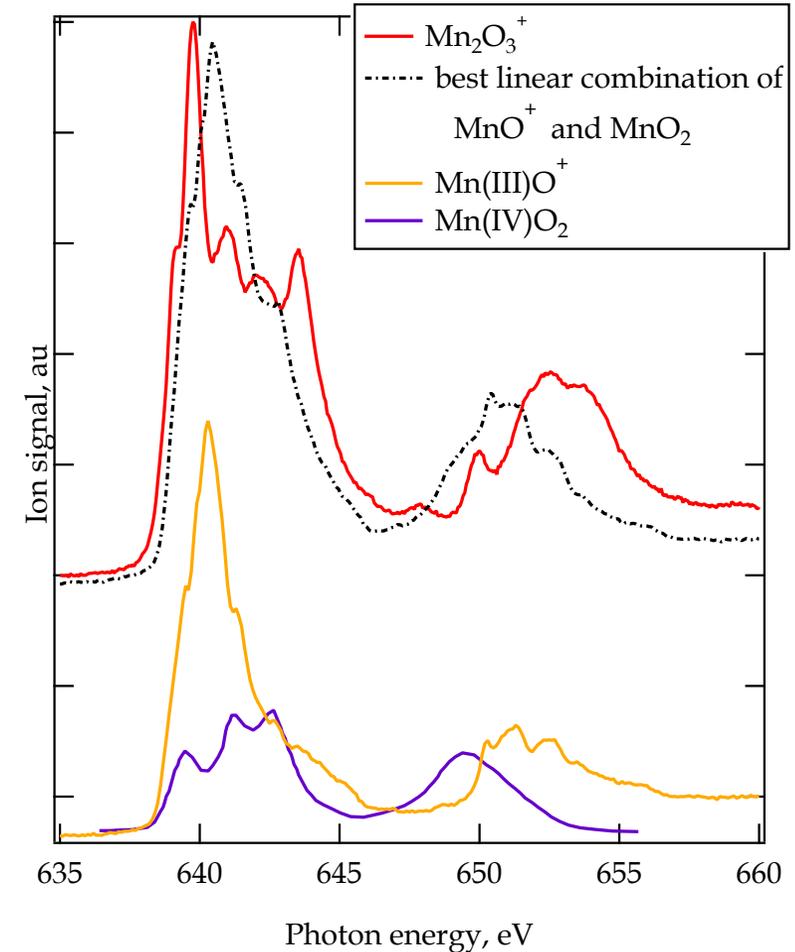
Oxidation states
II and V



$$\text{Cos Sim} = \frac{A * B}{\|A\| * \|B\|}$$

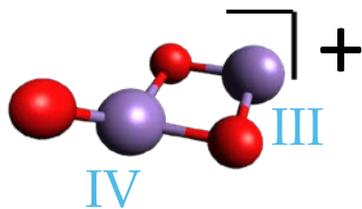
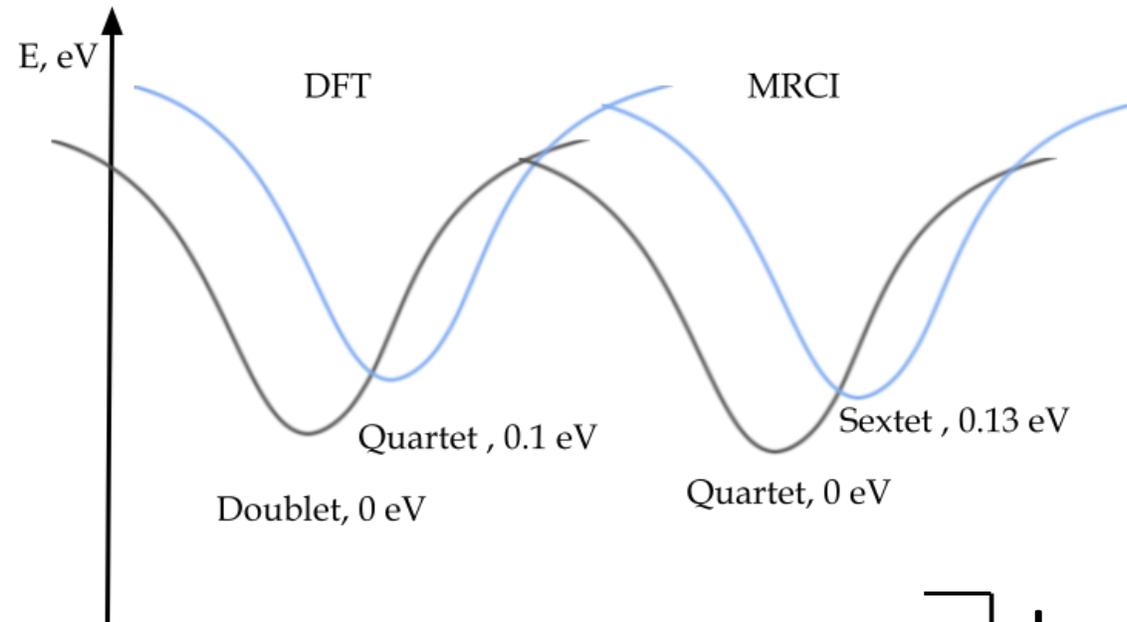


Cosine similarity 0.9898

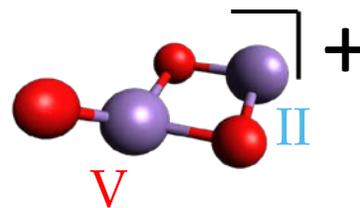


Cosine similarity 0.9454

Potential energy surface

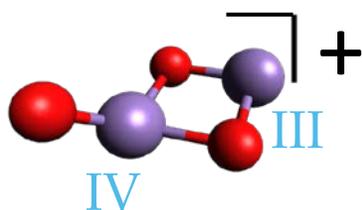
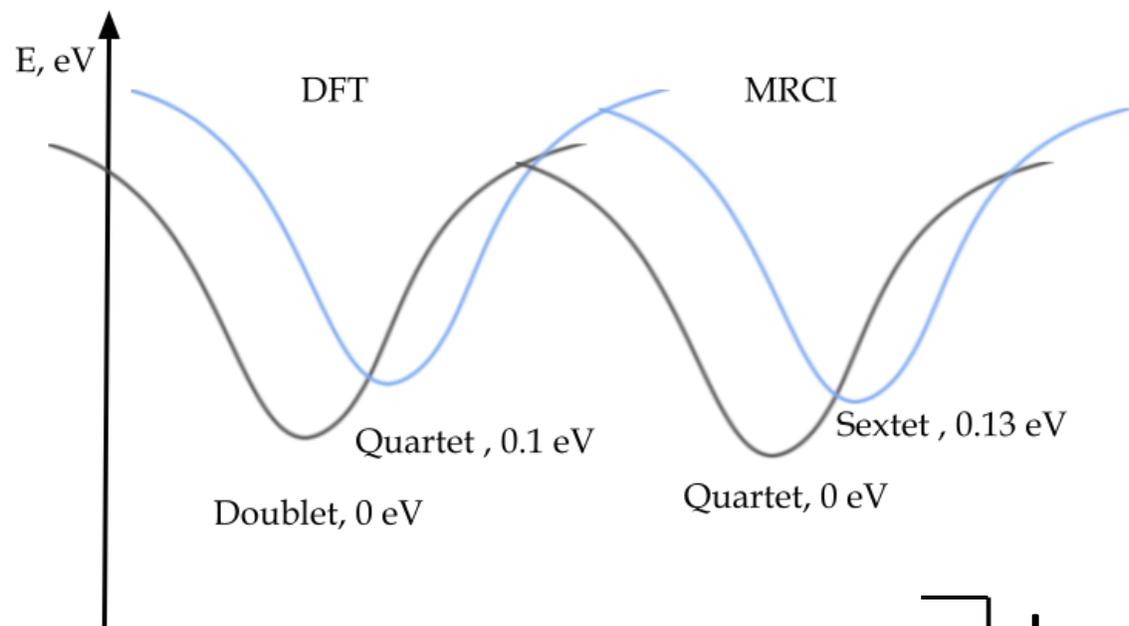


Method: TPSSh + D3BJ

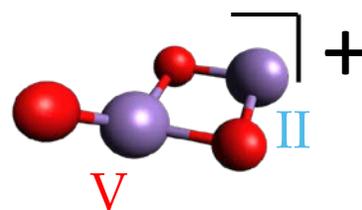


Method: CASSCF + SC/PC-NEVPT2

Potential energy surface

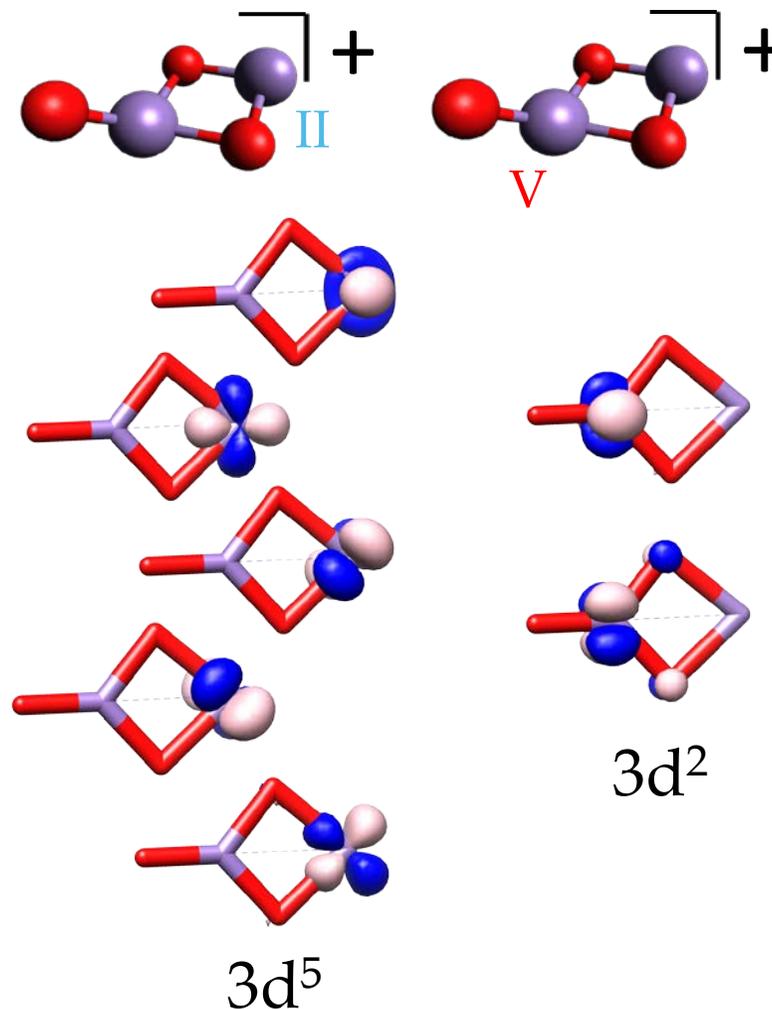


Method: TPSSh + D3BJ



Method: CASSCF + SC/PC-NEVPT2

Quartet



- ✦ We observed the Mn(V) oxidation state in a di-manganese system for the first time, which is a key to understand the nature of S_4 stage.
- ✦ Based on the Mn L-edge spectral signature we can assign the **oxidation state** of Mn atoms in $Mn_2O_3^+$ clusters
- ✦ For the proper description of the system with a high oxidation state of metal atom MRCI calculations is necessary, TD - DFT is not able to reproduce the ground state of $Mn_2O_3^+$
- ✦ $Mn_2O_3^+$ is the first step towards more complex system such as **$CaMn_4O_5$** .

A million thanks for our group and collaborator!

Department Highly Sensitive X-ray
Spectroscopy Helmholtz Zentrum Berlin

Prof. Tobias Lau



Quantum Chemistry of Complex
Molecular Systems Group from
Humboldt University

Prof. Michael Römelts

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DIY IN
RESEARCH
TRAINING
GROUP

C | A | M
DYNAMICS OF CONTROLLED
ATOMIC AND MOLECULAR
SYSTEMS

But if we will dig farther...