Properties of size selected sodium doped solvent clusters

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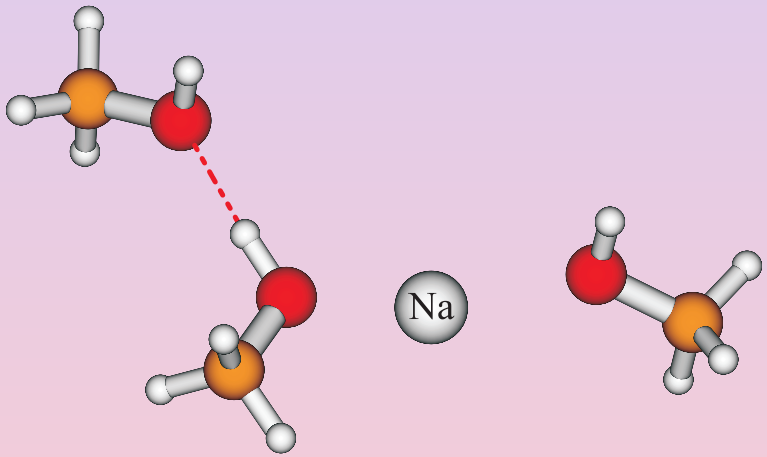
RF13 - Radicals and Ions

Outline



Motivation

Size dependent ionization potential (IP) of sodium doped solvent clusters:

Systems that have already been measured:

- sodium doped ammonia cluster[a,b] $Na(NH_3)_n$
- $\hookrightarrow$ show a strong size dependence of the IP
- sodium doped water cluster[b] $Na(H_2O)_n$
- $\hookrightarrow$ only show a size dependent decrease for clusters up to n=4, for larger clusters the IP is constant

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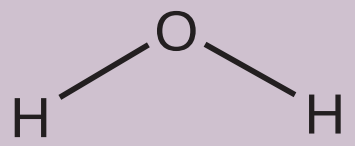
What is with other systems?

- methylated water $\Rightarrow$ methanol
- learn more about the properties and the structures of these clusters
- learn more about solvation of electrons



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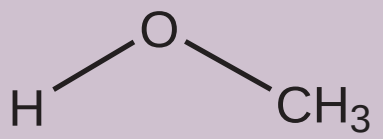

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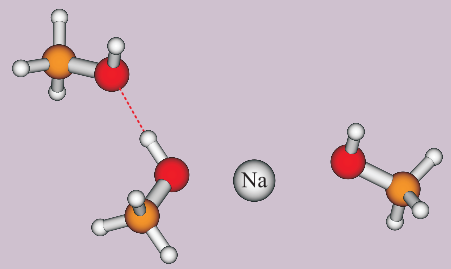

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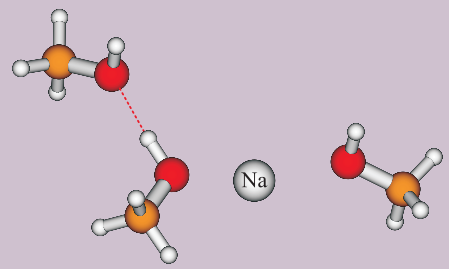

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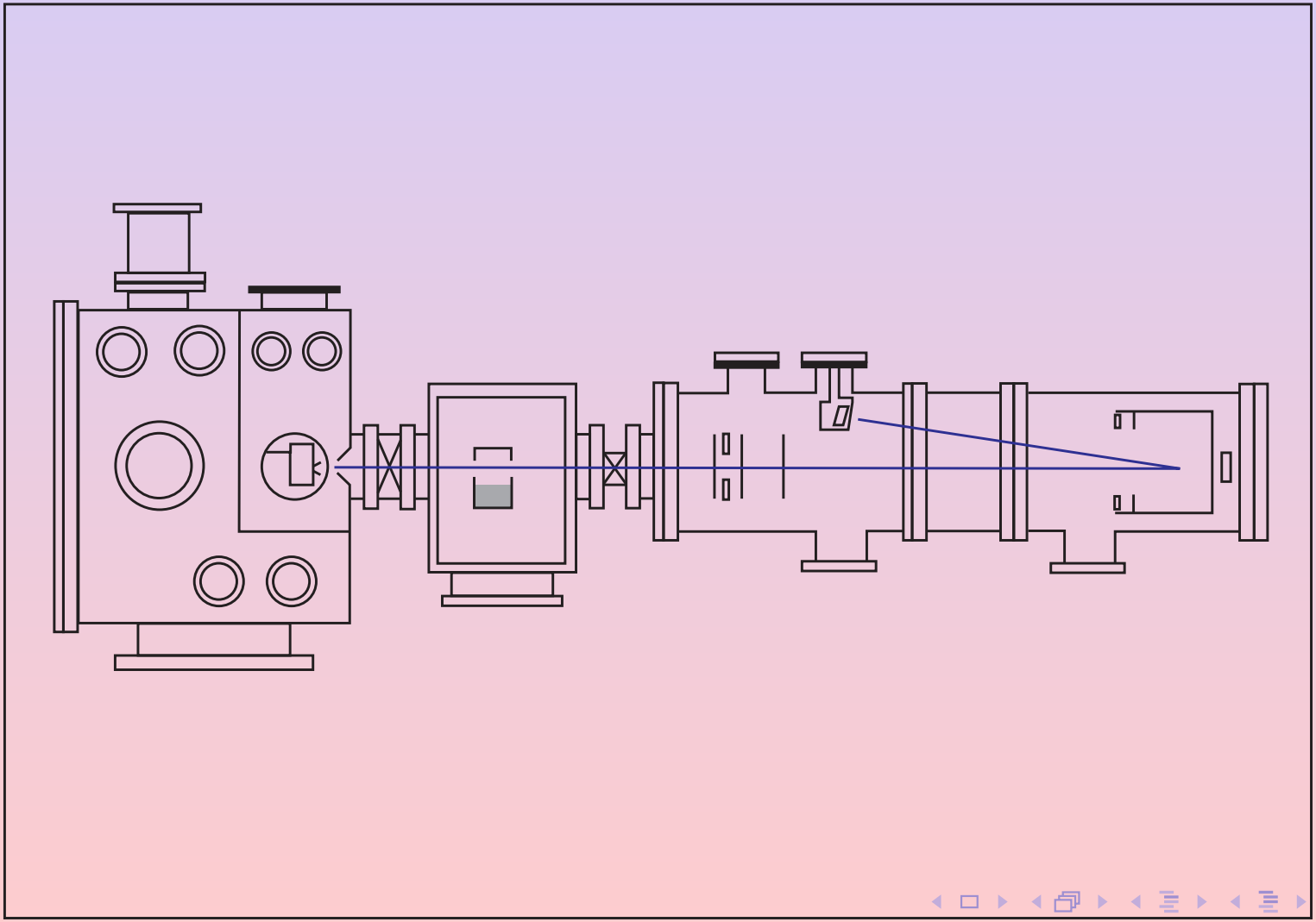
Experimental setup



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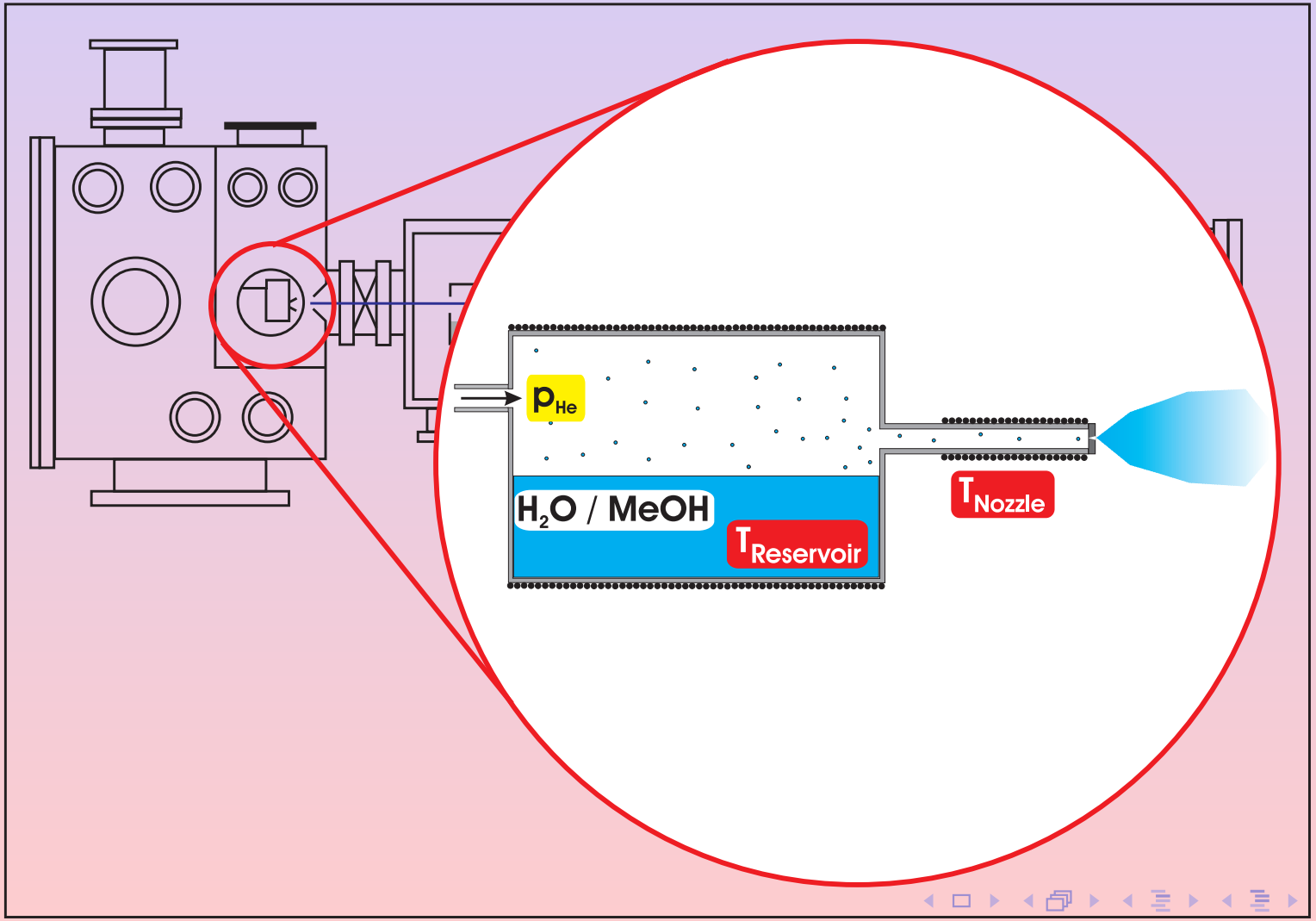

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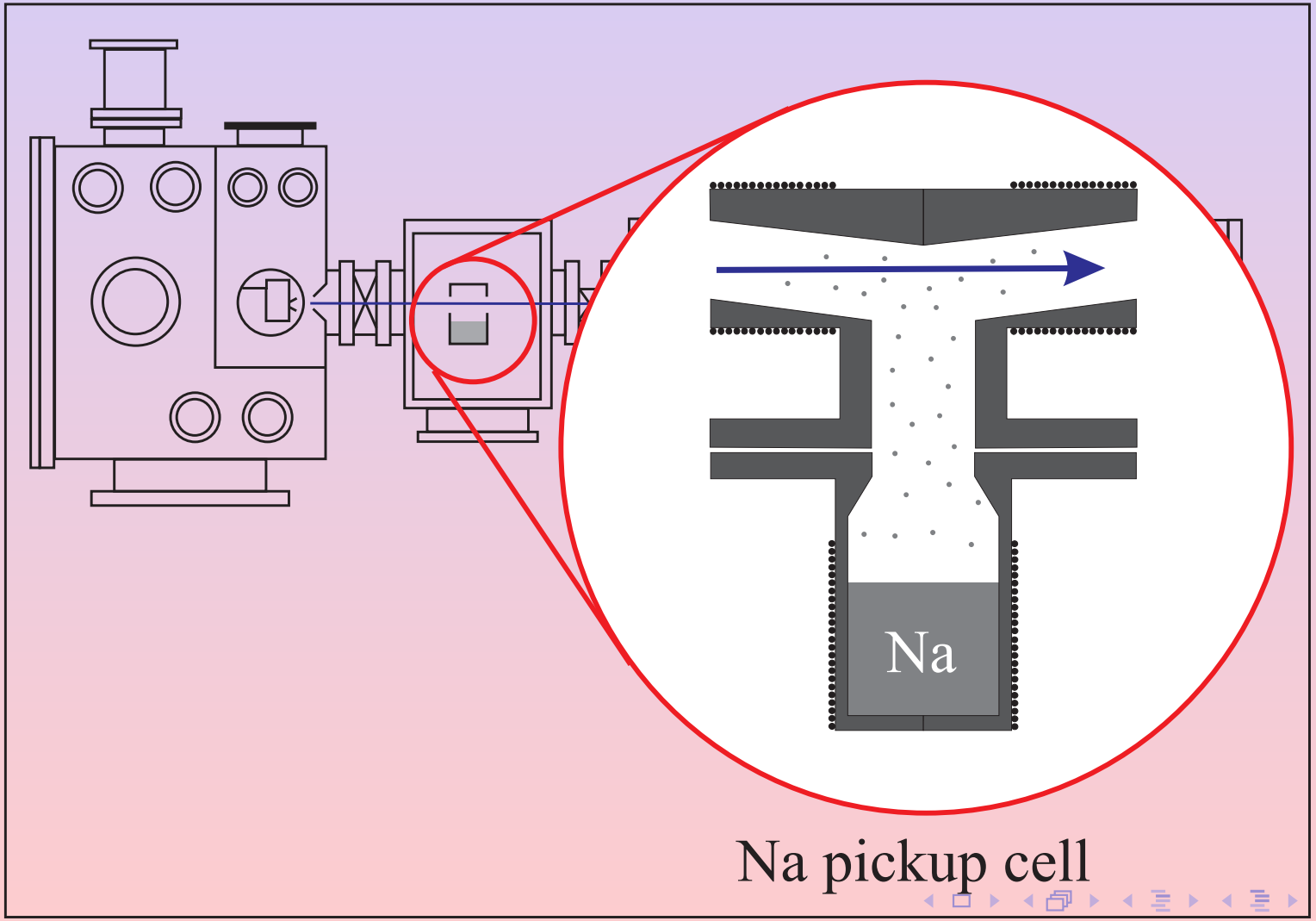
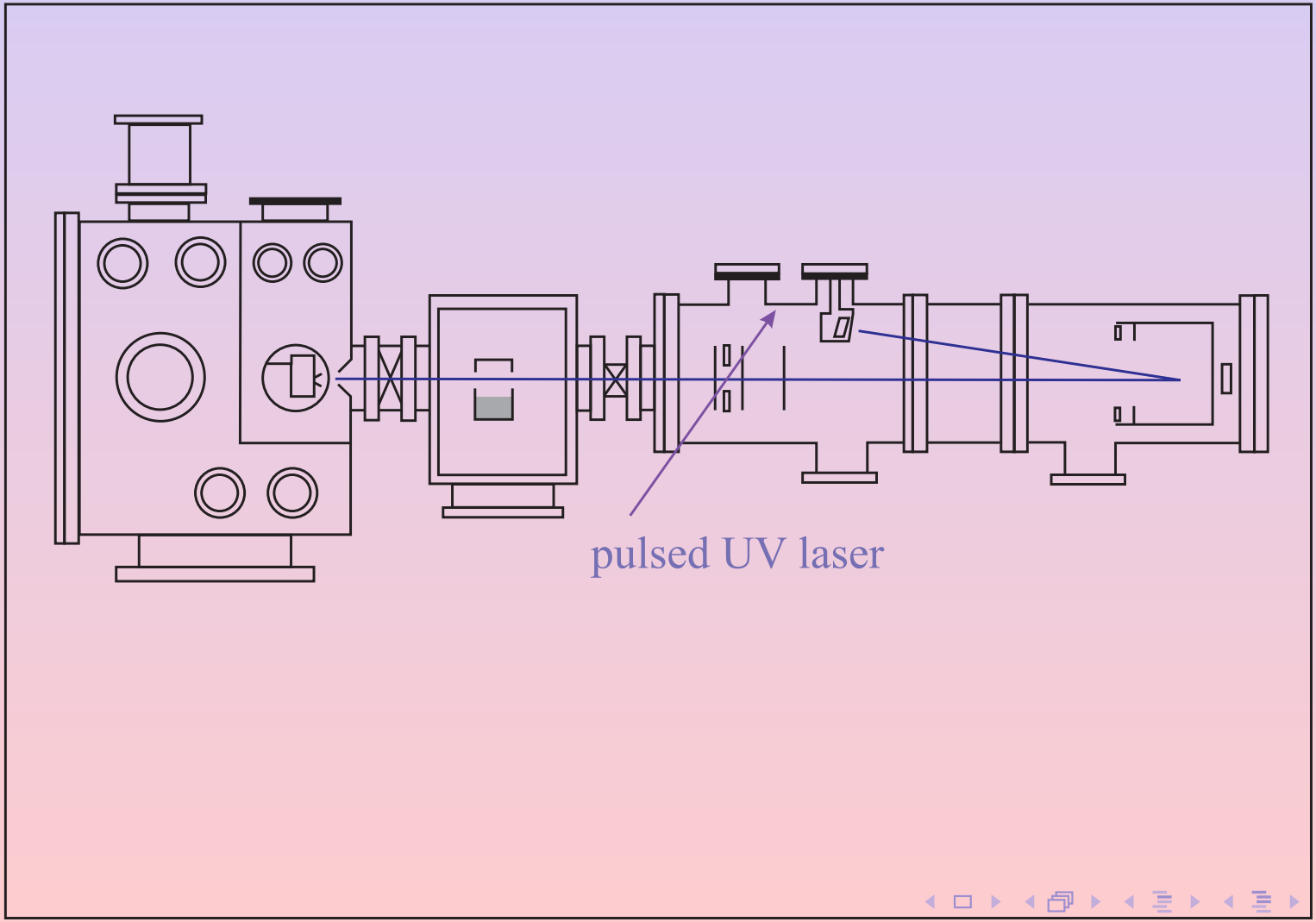
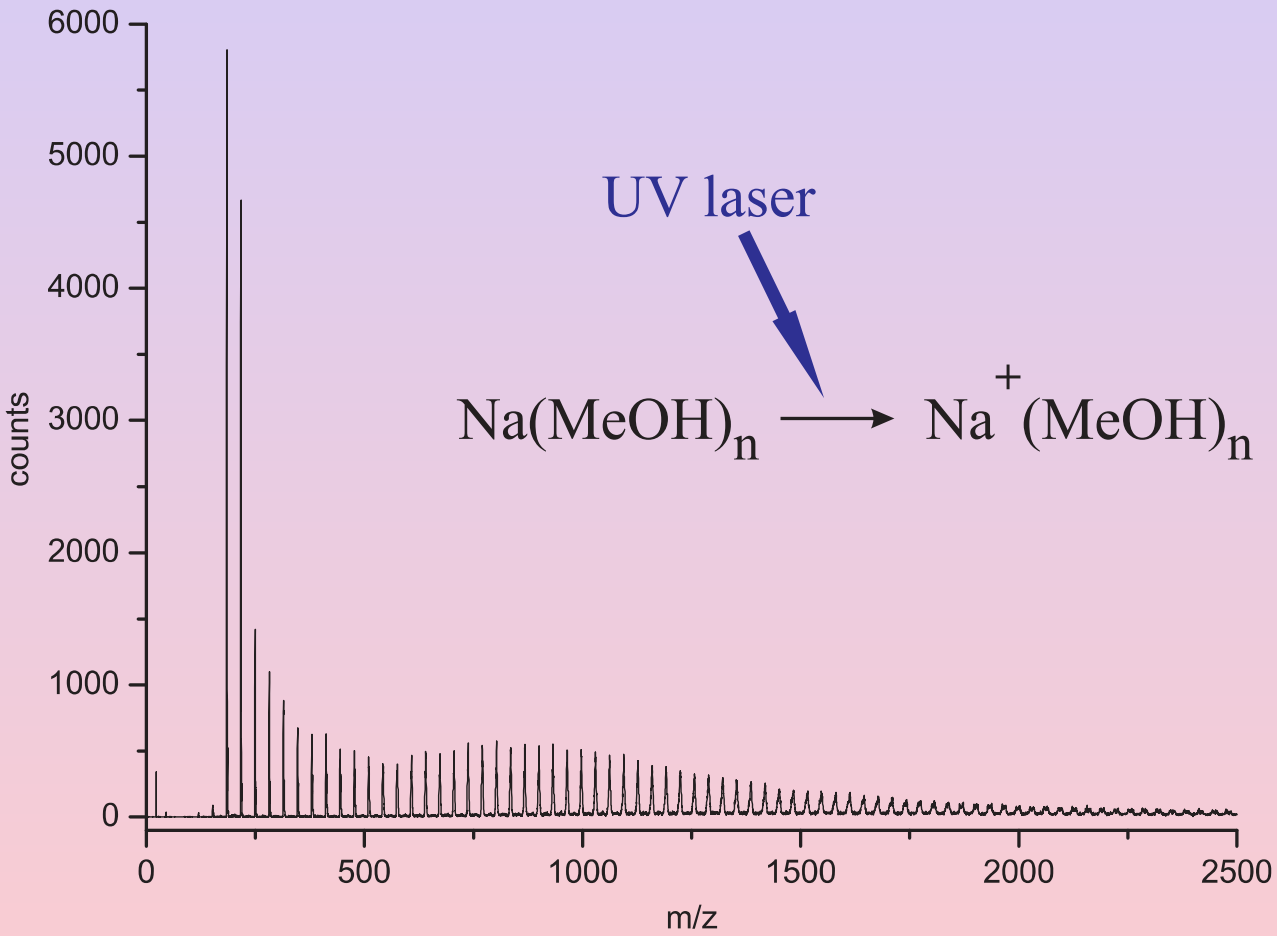


Na pickup cell

Experimental setup



Mass spectrum of $Na(MeOH)_n$



$\lambda_{ion} = 370$ nm

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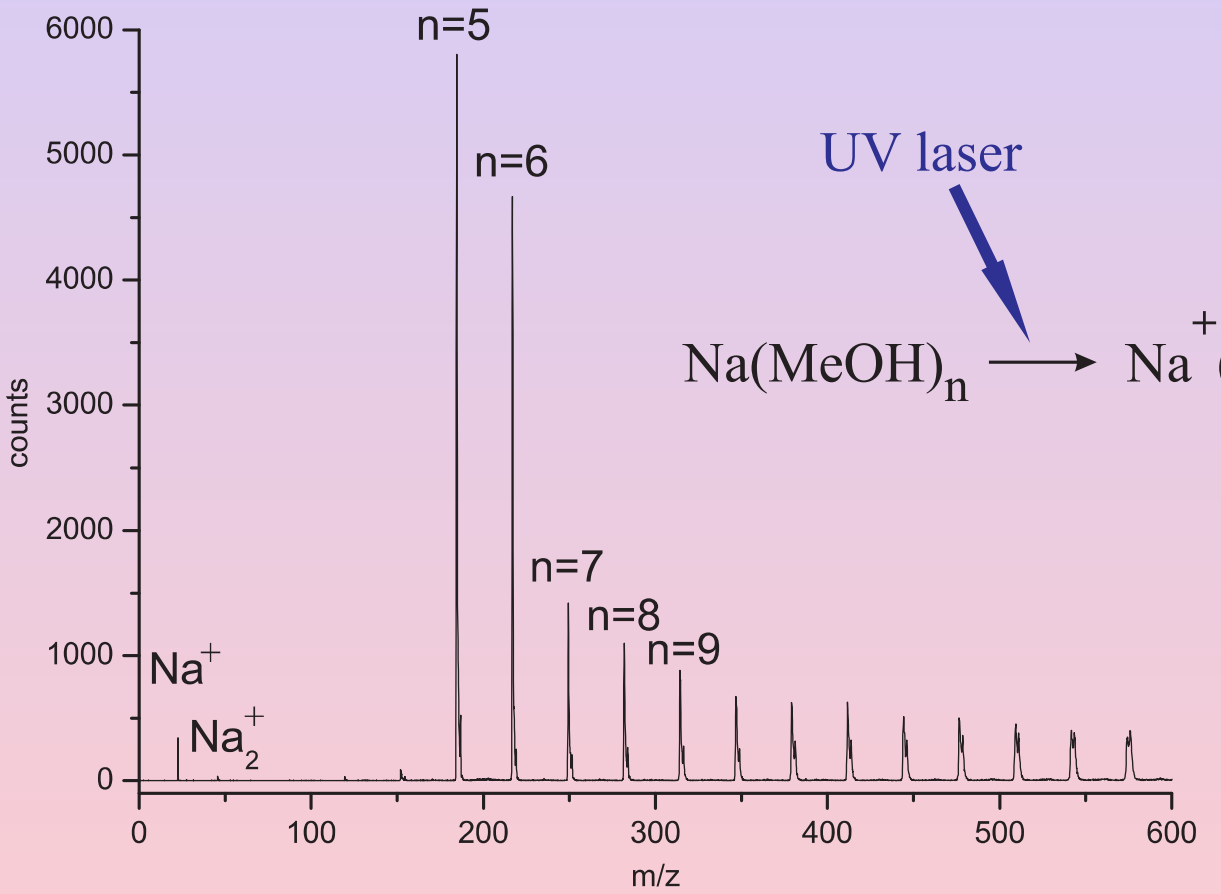


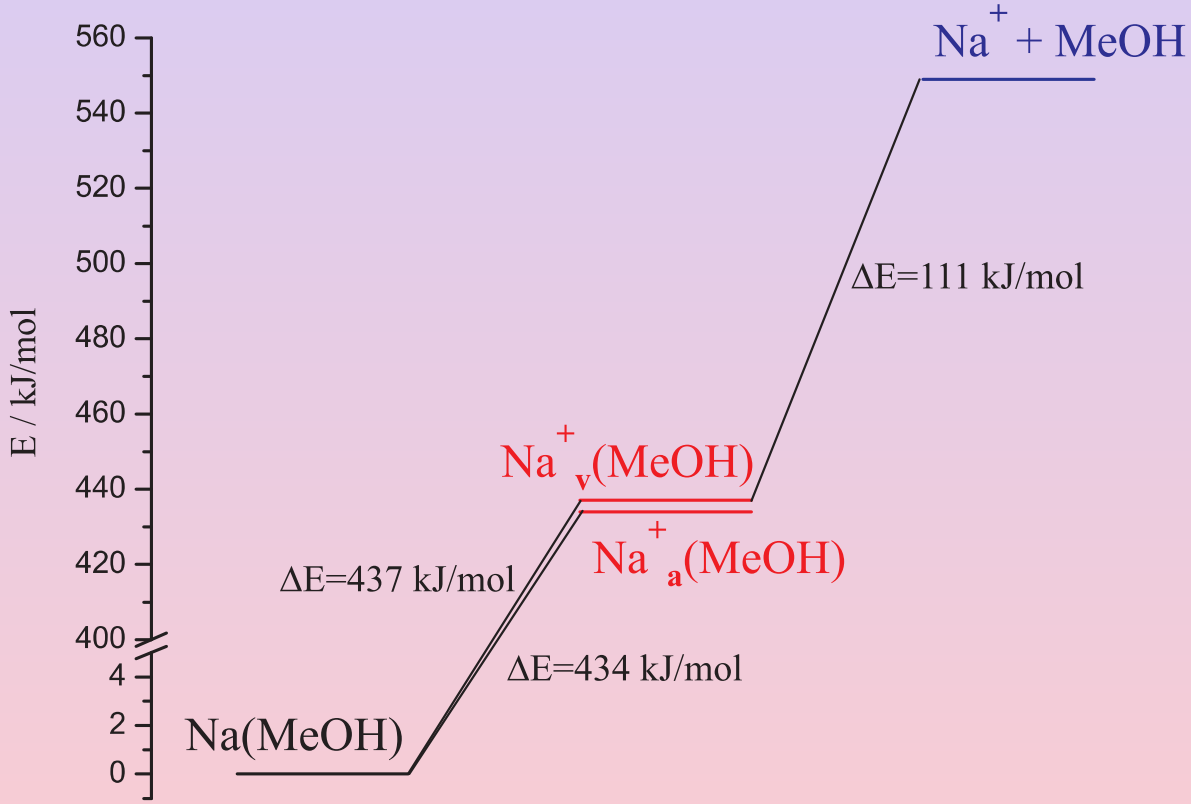
UV laser

$$Na(MeOH)_n \longrightarrow Na^+(MeOH)_n$$

$\lambda_{ion} = 370$ nm

DFT calculations

$Na(MeOH)_1$



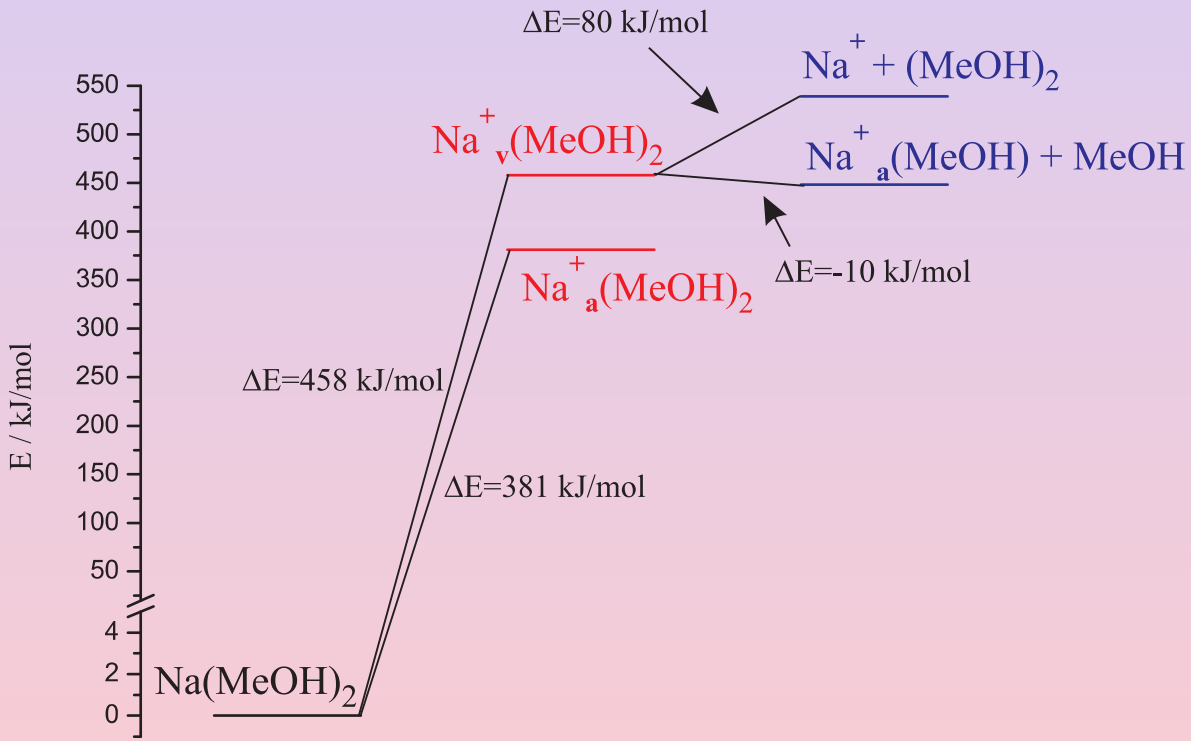
UB3LYP / 6-31+G(d,p)

$\Rightarrow$ no fragmentation

(Bing Gao and Zhi-feng Liu, Chinese University of Hong Kong)

DFT calculations

$Na(MeOH)_2$

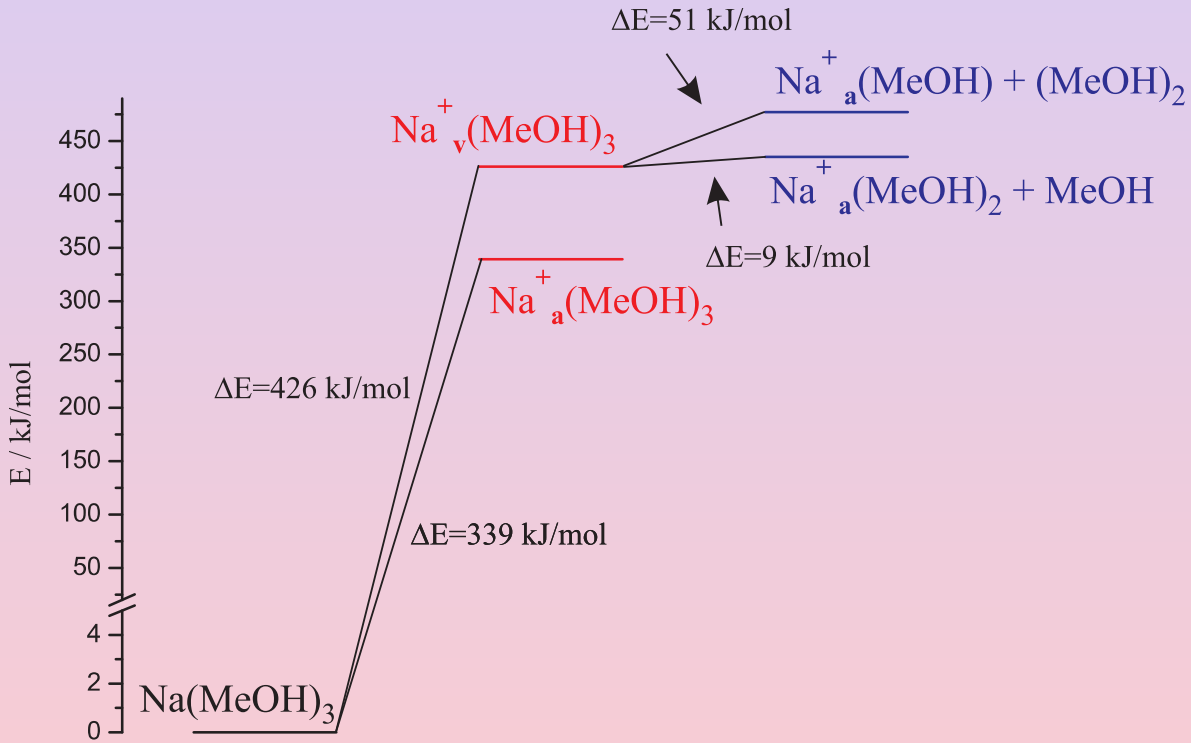


UB3LYP / 6-31+G(d,p)

$\Rightarrow$ no fragmentation

DFT calculations

$Na(MeOH)_3$



UB3LYP / 6-31+G(d,p) $\Rightarrow$ no fragmentation $\Rightarrow$ soft ionization

Outlook

- determination of the size selective IP of $Na(MeOH)_n$ is running
- more DFT calculations of bigger clusters
- size selectiv IR action spectroscopy of $Na(MeOH)_n$ clusters[a]

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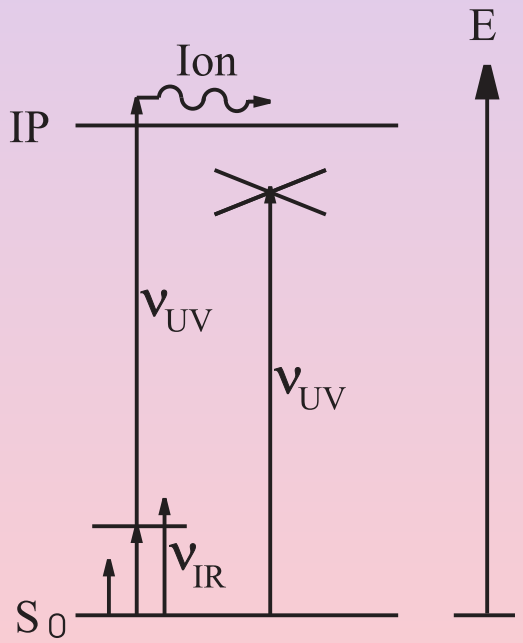

[a] C. Steinbach and U. Buck *J. Phys. Chem.* **110**, 2006, 3128–3131.

Acknowledgements

Financial support: GRK 782 of DFG
www.pcgg.de

Thank you for your attention!