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Jožef Stefan International Postgraduate School  
and Young Researchers' Day CMBO

*19 and 20 April*

## How do silanols react with oxidized aluminum surfaces?

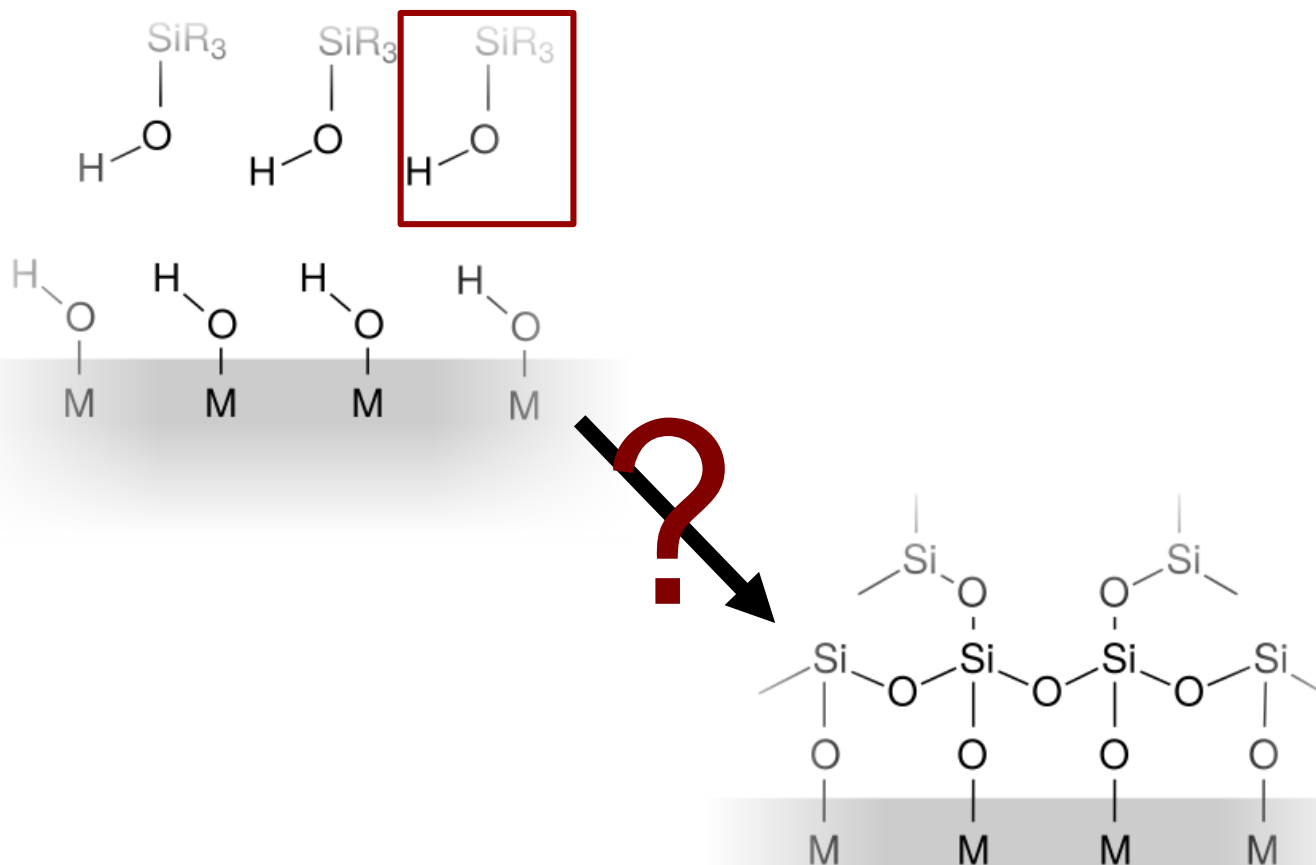
Matic Poberžnik,  
Jožef Stefan Institute  
Poster number: 7

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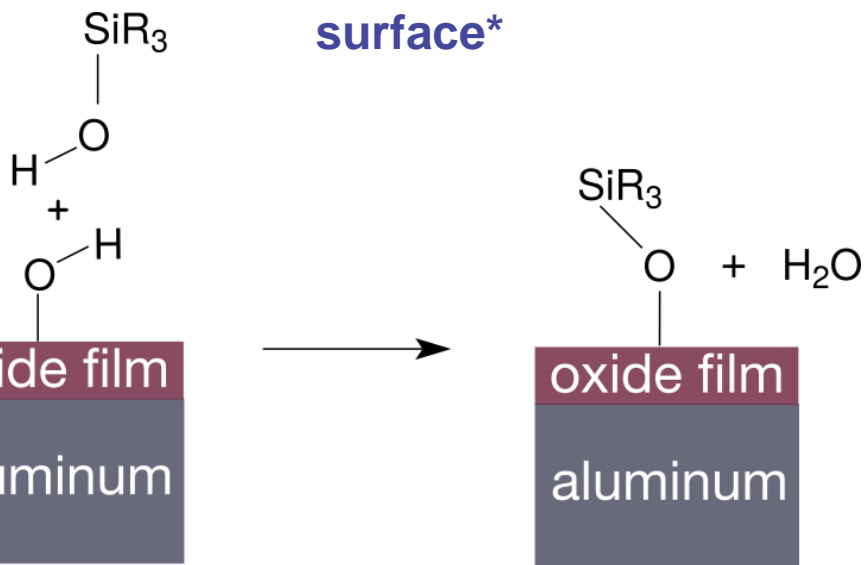
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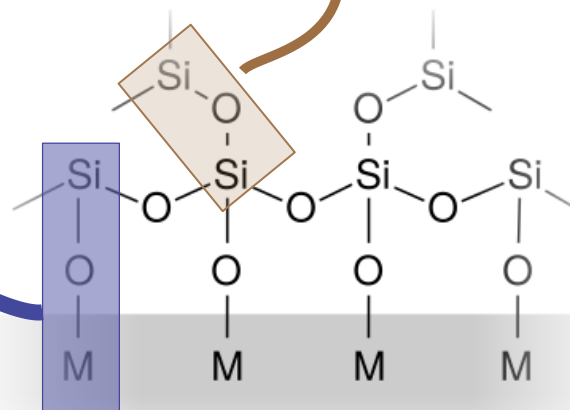
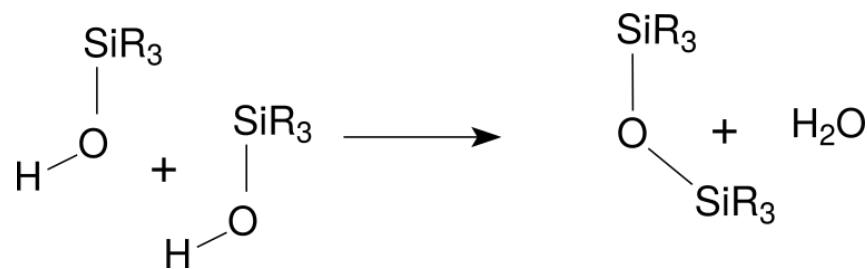


## Condensation reaction with aluminum surface\*



\*note: aluminum surface is oxidized upon exposure to the atmosphere or aqueous environment

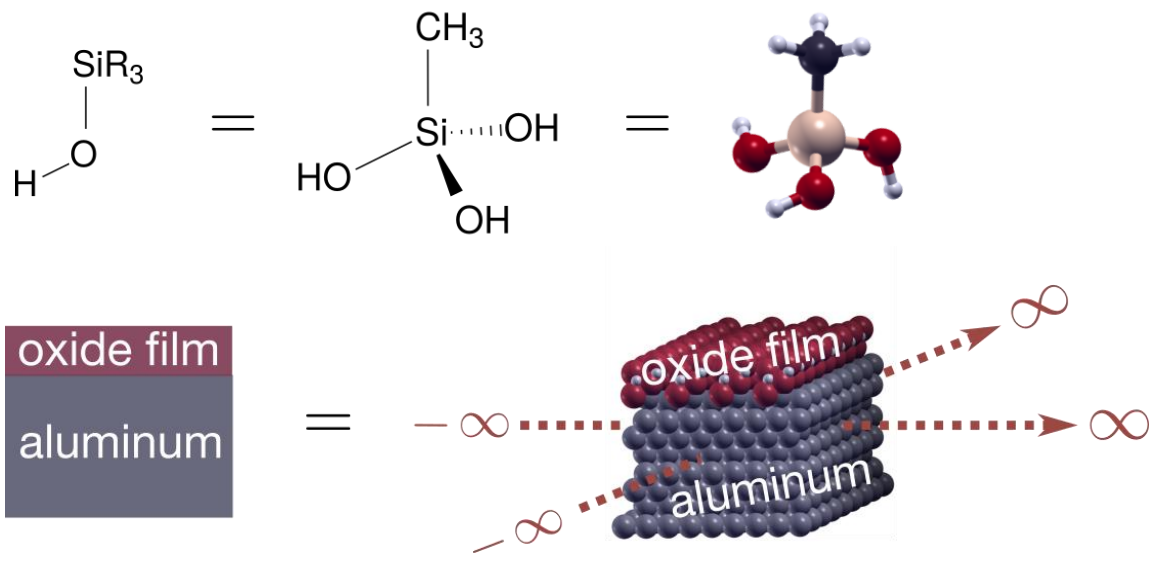
## Condensation reaction between two silanols



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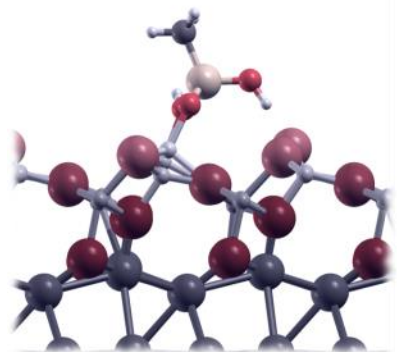
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$$\Delta E < 0?$$

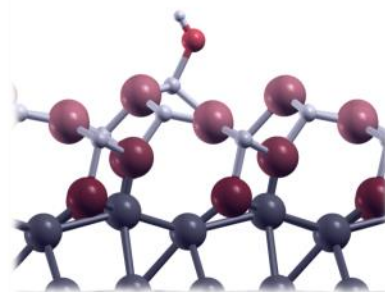
$$\Delta E = E_{\text{surface+silanol}} + E_{\text{H}_2\text{O}} - E_{\text{surface+OH}} - E_{\text{silanol}}$$



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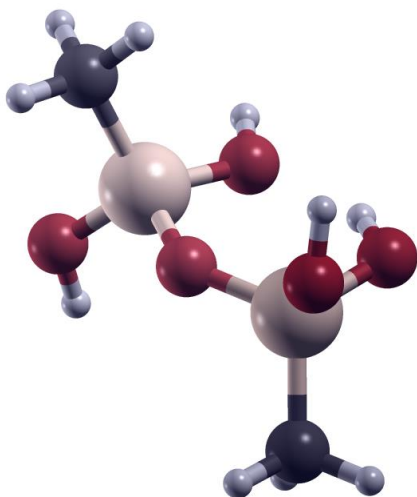
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$$\Delta E = E_{\text{products}} - E_{\text{reactants}}$$

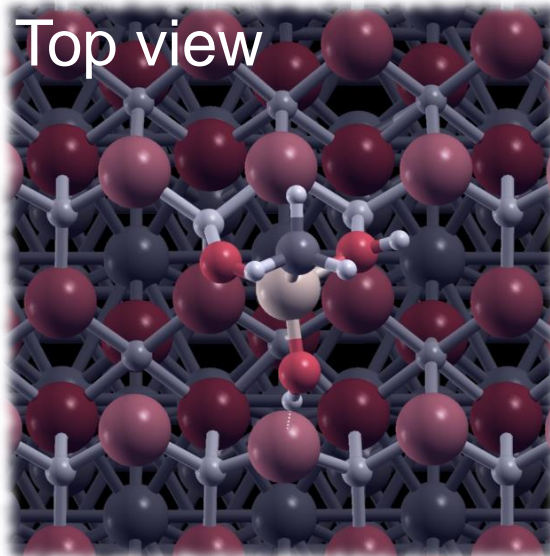
silanol+silanol



$$\Delta E_{\text{gas}} \approx \Delta E_{\text{water}}$$

$$\Delta E = -0.3 \text{ eV}$$

silanol+surface



Side view

$$\Delta E_{\text{gas}} = -0.8 \text{ eV}$$