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Augmented Reality Chemistry

Supporting Internal Model Representation in Organic Chemistry by Using Augmented Reality

Dr. Sebastian Habig
Chemistry Education

5th international
AR VR Conference
06/14/19

Motivation

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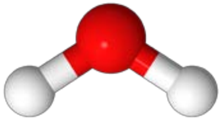
- In each STEM domain different kinds of representations are used to illustrate domain-specific concepts
  (e.g. Gilbert, 2007)

- There is a huge number of different representations in chemistry and instruction strongly relies on visualizations to illustrate important concepts
  (Gilbert, 2008; Rau, 2017; Treagust & Tsui, 2013)

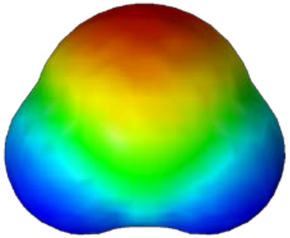
H_2O

molecular formula

Lewis structure



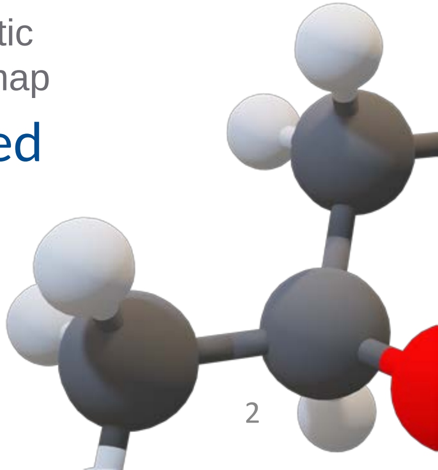
ball-and-stick model



electrostatic potential map

- Learning achievement in chemistry is positively correlated with spatial ability
  (e.g. Wu & Shah, 2004)

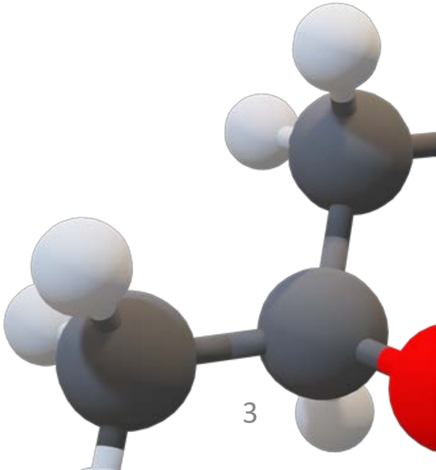
Chemists don't make it easy for novices to learn



Representations in Chemistry Education

- Dealing with scientific representations is a key component of chemistry studies
  (Coll & Lajium, 2011; Harrison & Treagust, 2000; NRC, 2006)
- Cognitive processing multiple external representations is crucial for the learning of new concepts
  (Baker & Talley, 1972; Wu & Krajcik, 2006; Wu & Shah, 2004)
- For many students (especially novices) it is difficult to extract information from external representations which is relevant for their learning process
  (Oliver-Hoyo & Sloan, 2014; Rau, 2017)

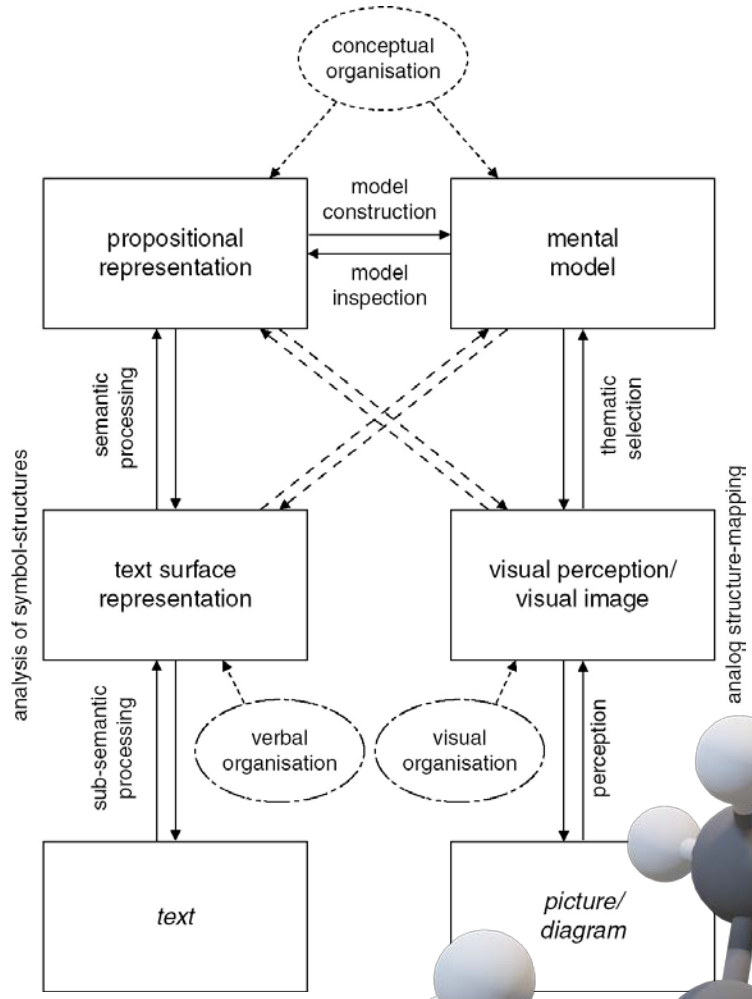
⇨ *Representation dilemma* (Rau, 2017)



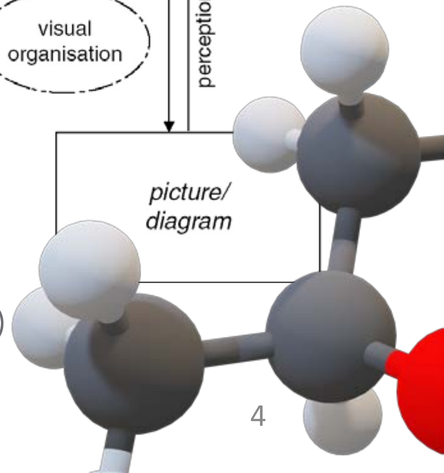
Representations in Chemistry Education

- CTLM (Mayer, 2009, 2014)
  ITPC (Schnotz, 2014)
- Multiple external representations can promote learning
- Simultaneous processing of textual and visual information
- High demands on spatial skills in Chemistry may lead to cognitive overload

  Gender differences in mental rotation ability in favor of males
  (Harle & Towns, 2011; Kimura, 2000; Terlecki & Newcombe, 2005; Voyer et al., 1995)



(Schnotz & Bannert, 2003)



Example:
Nomenclature of Absolute Configuration

Carbon C2 is the chirality center of 2-butanol. The sequence of CIP rank for the substituents of C2 is: hydroxy group (A) (atomic number of oxygen is 8), ethyl group (B) (atomic number of carbon is 6 and a further carbon in the second sphere), methyl group (C) (atomic number of carbon is 6 but only hydrogens in the second sphere), and finally the hydrogen (D) (atomic number of hydrogen is 1).

2-butanol

enantiomer I   enantiomer II

Fig.1

Subsequently, one looks at the molecule in the direction of the bond between the chirality center (C2) and the substituent of the lowest CIP priority (H (D)) from the opposite side of this substituent. For this purpose, the molecular model is orientated such that the substituent of lowest CIP priority is covered with the chirality center. Then, the three substituents of higher priority form a triangle (A,B,C) around the chirality center. Try to orientate the interactive molecular models below with your mouse so that you can see the triangle (A,B,C).

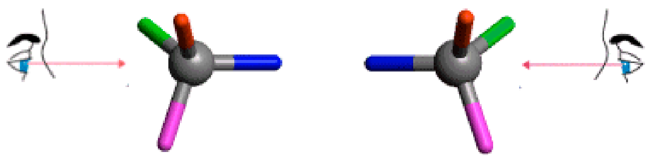


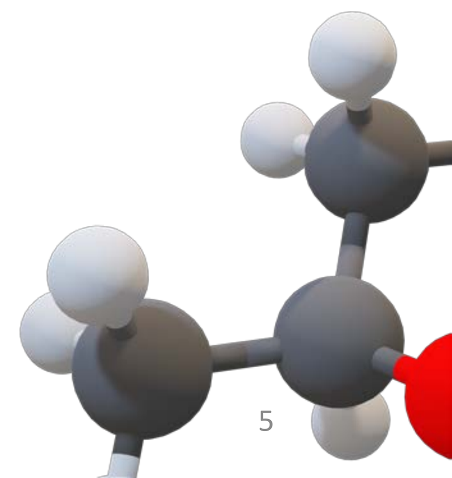
Fig.2

Source: chemgapedia.de

Textual and symbolic representations

Multiple external representations

Spatial 3D information



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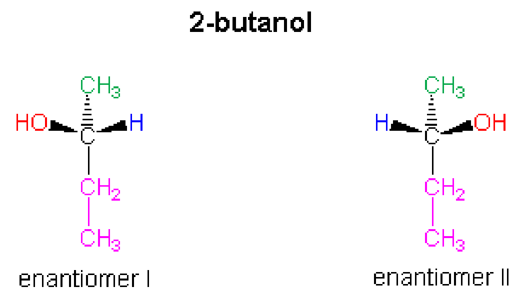

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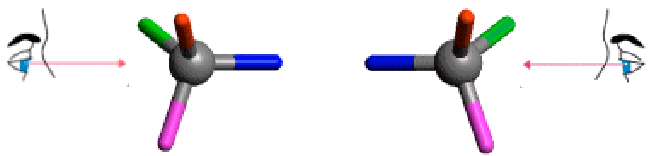
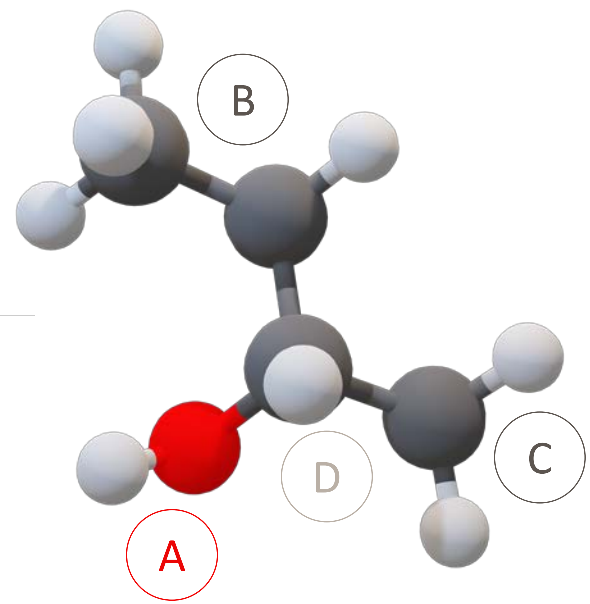


Fig.2



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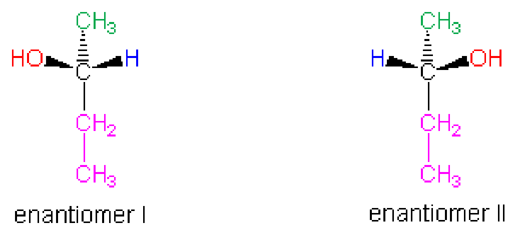
2-butanol



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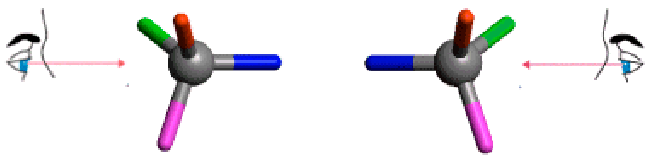

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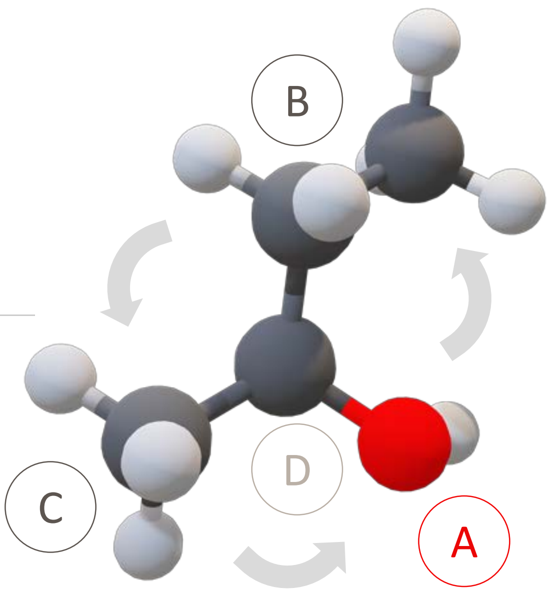

(2S)-2-Butanol

Source: chemgapedia.de

Augmented Reality as Instructional Tool

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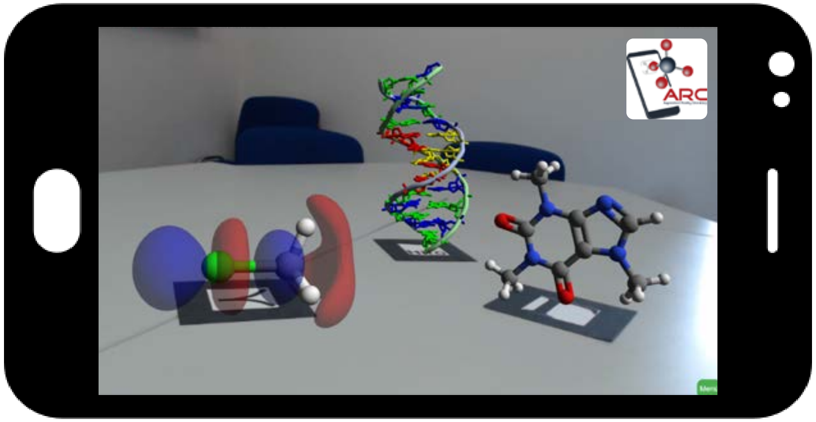
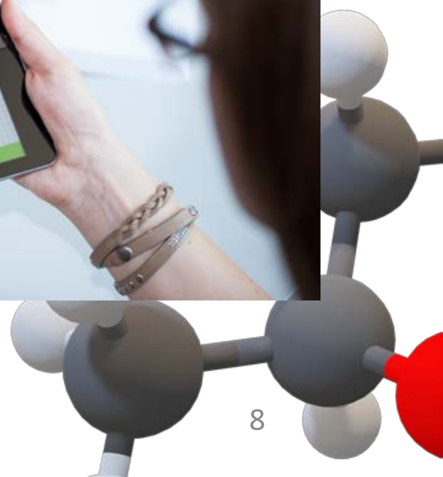
The integration of three-dimensional, virtual objects in real environments in real-time

(Azuma, 1997)



App Augmented Reality Chemistry

- Combining conventional text-based instruction and interactable 3D AR models and animations
- Visualize ball-and-stick models, atom- and molecular orbitals or complex molecular structures



Potential of Augmented Reality in Educational Settings

(Bacca et al., 2014; Ibáñez & Delgado-Kloos, 2018; Radu, 2014)

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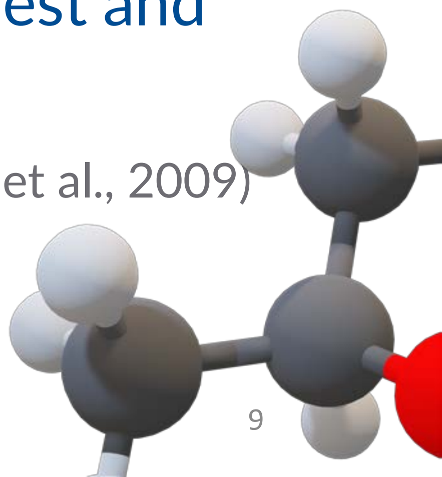
Positive effects on learning achievement

- By the possibility to visualize **complex, three-dimensional** concepts (e.g. Arvanitis et al., 2009; Bitter & Corral, 2014)
- By the possibility to illustrate **non-visible phenomena** or technical processes (e.g. Klopfer & Squire, 2008)
- By **reducing cognitive load** (e.g. Cheng & Tsai, 2013)

Promoting affective factors of students (e.g. interest and motivation)

- Mediated by usability (e.g. Choi & Baek, 2011; Dunleavy et al., 2009)
- Possible novelty effect (e.g. Akçayır & Akçayır, 2017)



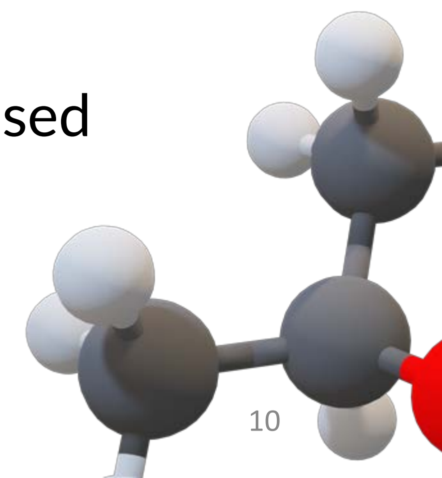
Aim of the Study and Research Questions

- In a first step we want to investigate if chemistry students are able to use AR representations to solve domain specific tasks.
- In this study we focus on the absolute configuration of chemical structures.

RQ1:
Do students determine the absolute configuration of chiral molecules more often correct when AR representations are provided?

RQ2:

Do females benefit to a higher degree from AR-based visualizations than males?



Study Design

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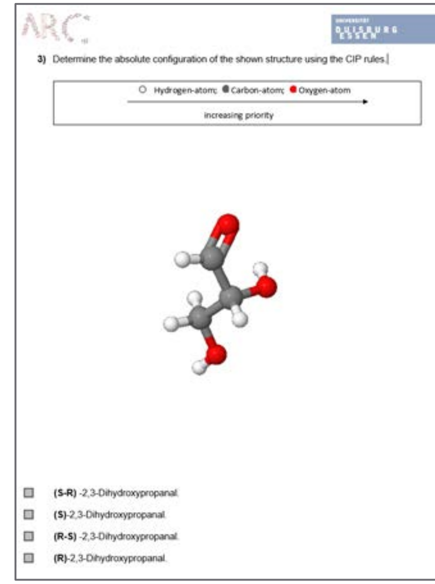
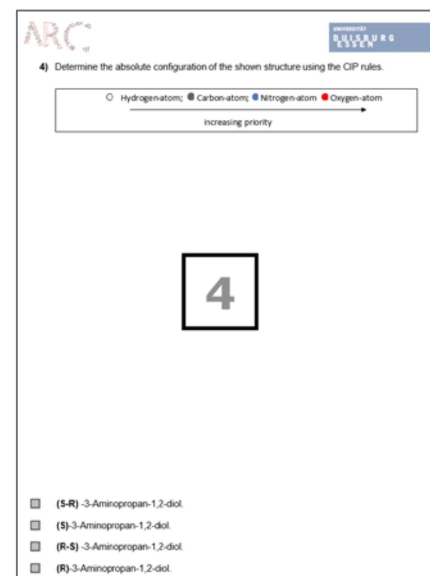
Stereoisomer-Test (paper-pencil)

- 14 items on determining the absolute configuration of a given structure using the CIP rules
- 7 ball-and-stick visualizations
- 7 AR visualizations
- The students were able to visualize the AR models with the help of a provided tablet-pc
- Multiple-choice-single-select format
- $\alpha_{Cronbach} = .70$





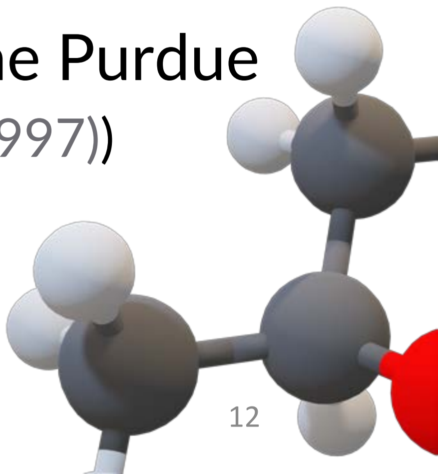
Sample & Control Variables

Sample

- *N*=31 (16 female) college students who were enrolled in a bachelor chemistry program completed the test
- Part of their regular advanced organic chemistry course (90 minutes)
- The students were familiar with the CIP rules

Control Variables

- Mental rotation ability (shortened version of the Purdue Visualization of Rotations Test (Bodner & Guay, 1997))
- Rating scale '*general use of media*' and '*AR Experience*'



Results (Habig, 2019)

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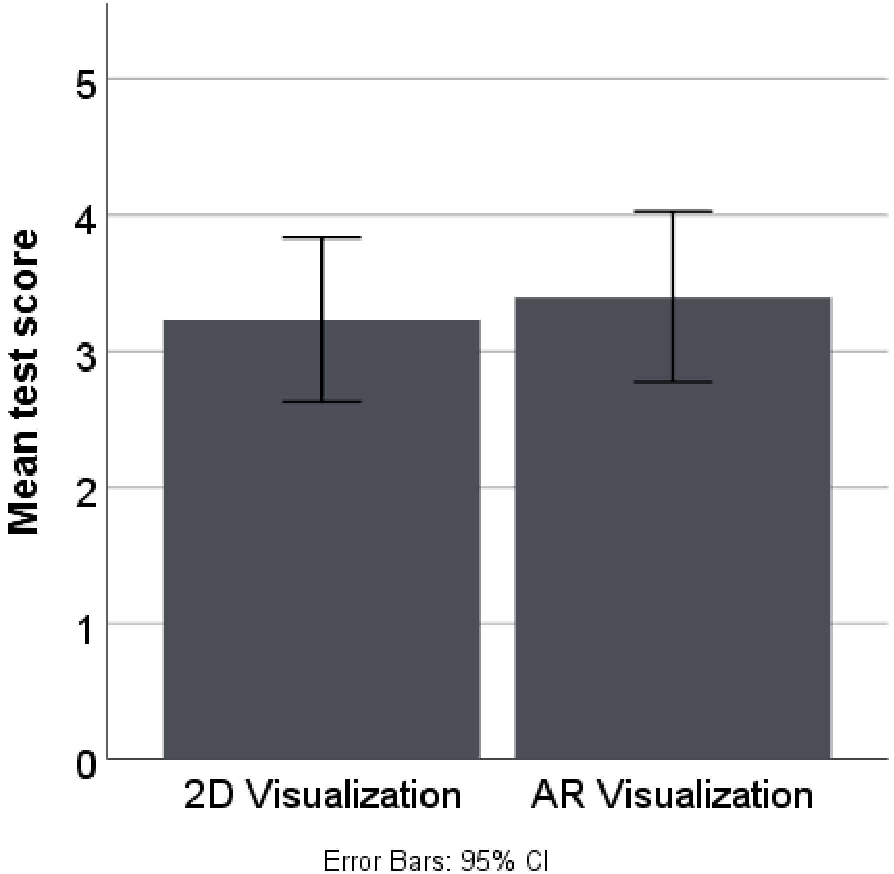
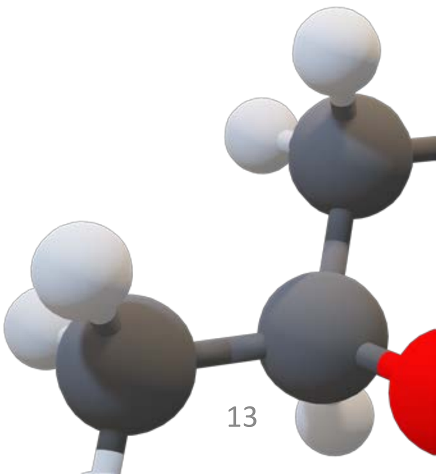
Do students determine the absolute configuration of chiral molecules more often correct when AR representations are provided?



No statistically relevant differences in test scores

($t(29) = 0.542$, $p = .59$)



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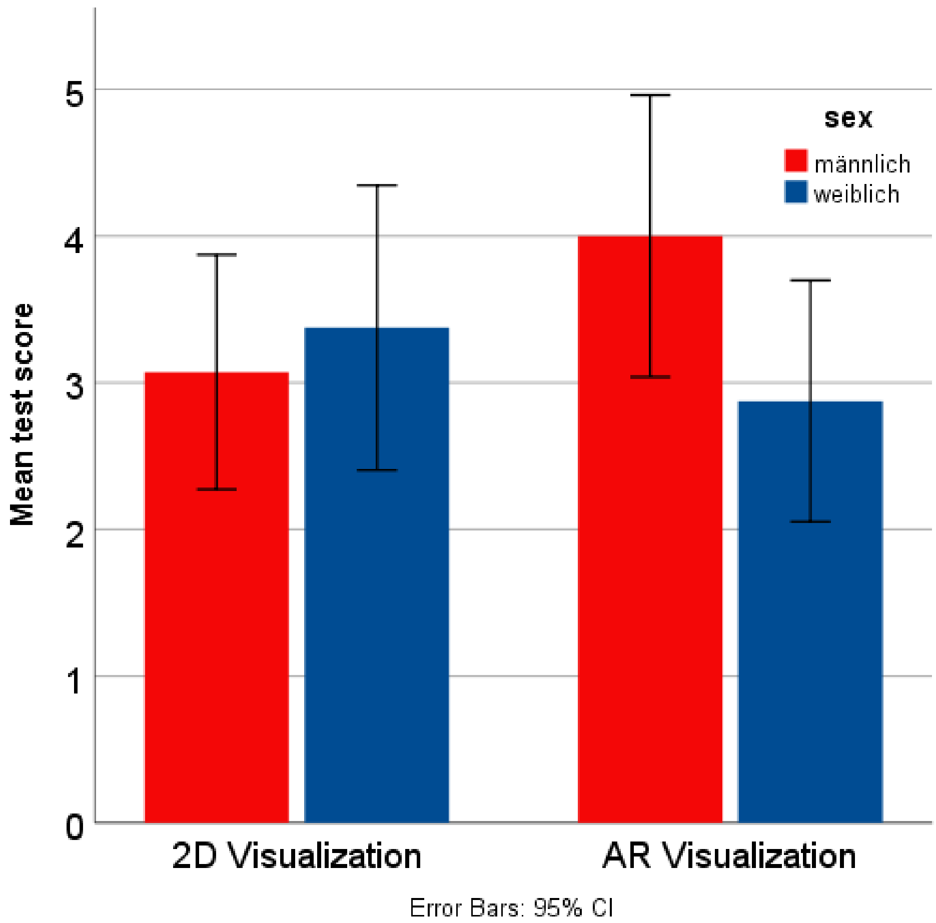
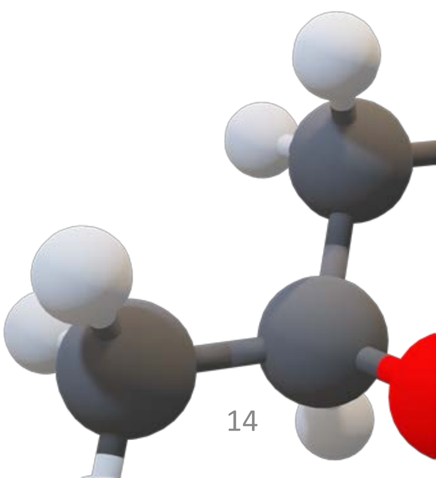
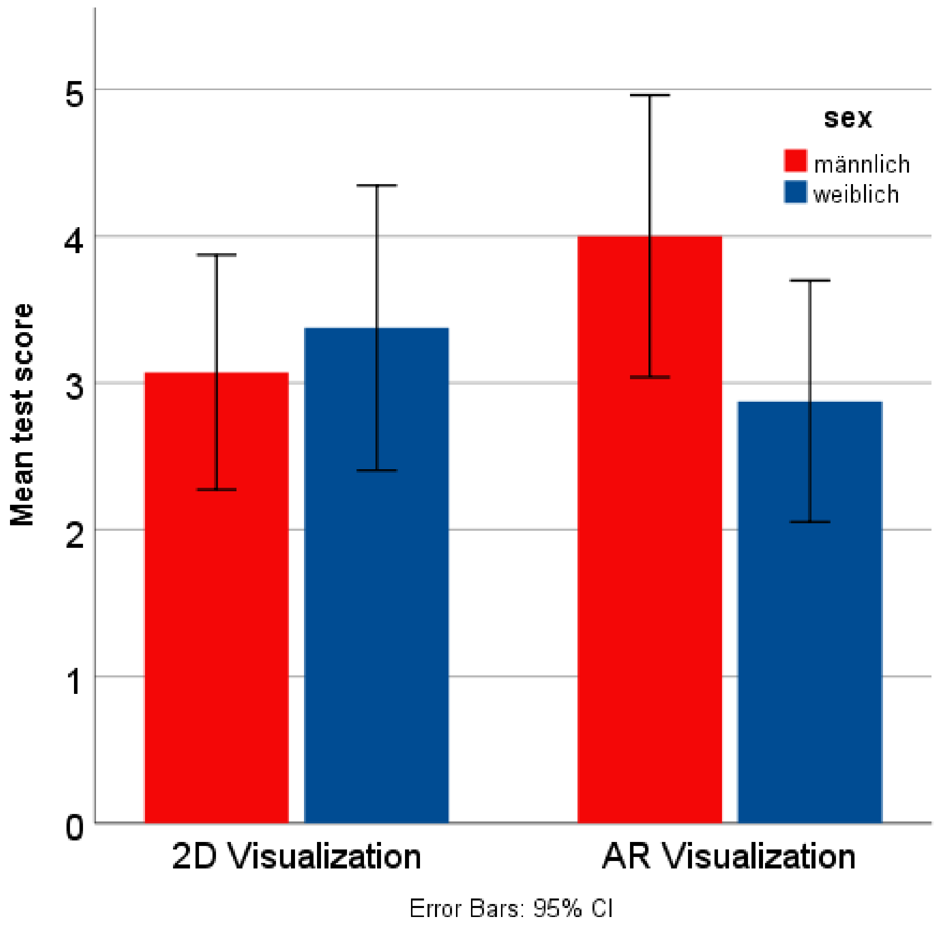


Do females benefit to a higher degree from AR-based visualizations than males?

- Effect of gender
  ($F(1, 28) = 6.375$, $p = .018$, $d = .95$)
- On average males score higher on the AR part of the test
- On average females score higher on the 2D part of the test



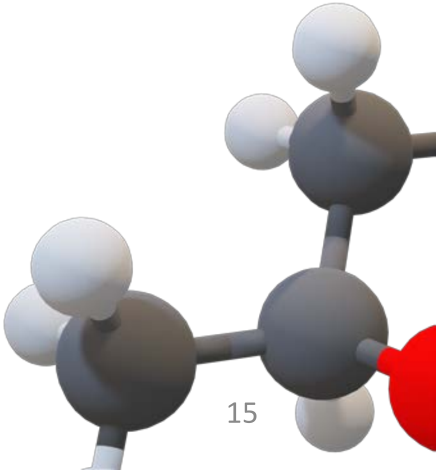
Results (Habig, 2019)



Do females benefit to a higher degree from AR-based visualizations than males?

- Effect of gender (controlled for mental rotation ability)

  ($F(1, 27) = 8.497$, $p = .007$, $d = 1.12$)



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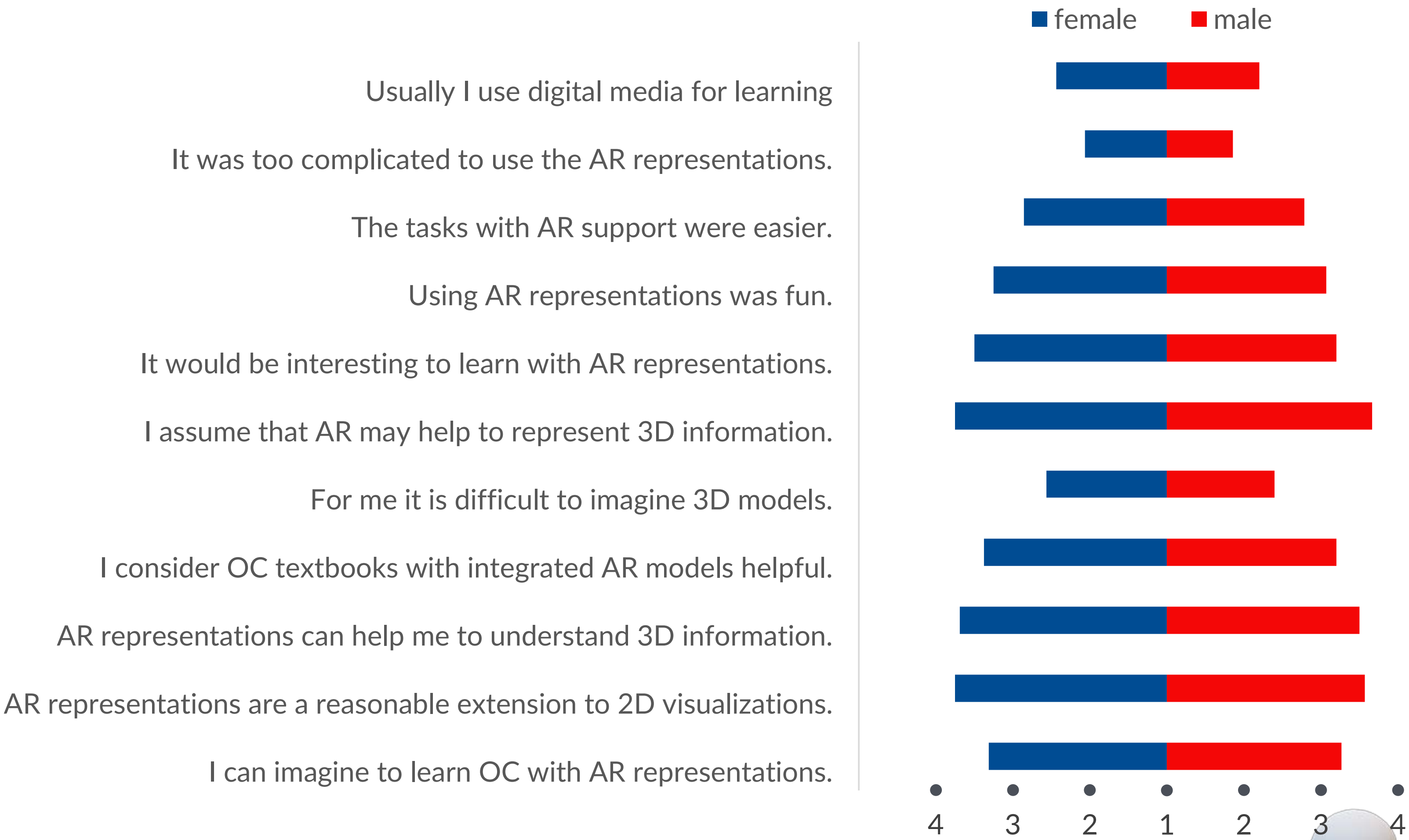

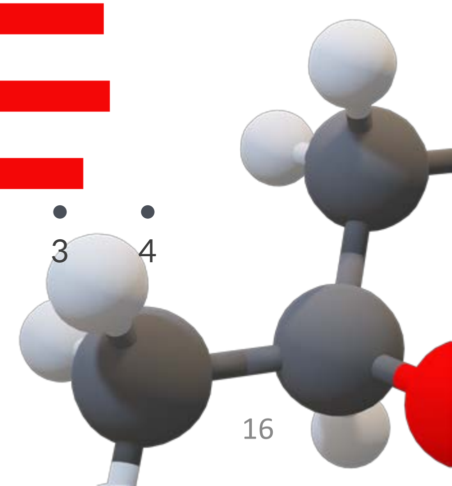

Discussion & Implications

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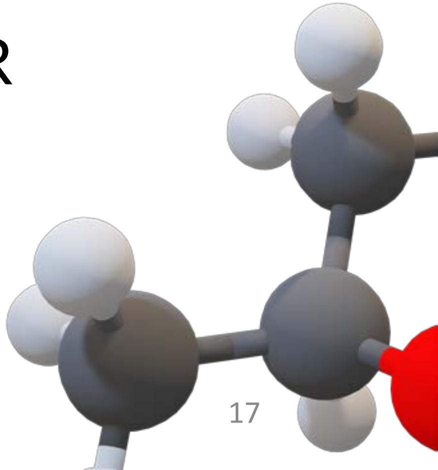
- Effect of Gender raises new questions

⇨ A reason for the found differences may be that using digital resources which require spatial abilities is more prevalent among males than females. (Doyle, Voyer, & Cherney, 2012; Feng, Spence, & Pratt, 2007)

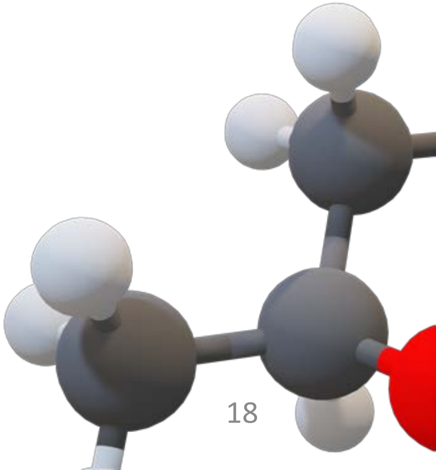
⇨ Further research should focus on cognitive and affective learner characteristics and how they influence learning with AR.

⇨ Provide a training on how to properly use AR representations



Limitations

- Small sample size
- Limited to an assessment setting
- Only one content area
- No measure of cognitive load



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Thank you for your attention!

Suggestions, Questions, Ideas?

Contact:

Dr. Sebastian Habig

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