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Coding & digitalization in physical chemistry to enhance learning outcomes and digital skills

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Mastering digital skills is more important than ever as digitalization infiltrates every aspect of our lives in general and the scientific process in particular. The evaluation of experimental data, laboratory journals, reports in universities and industry are now all digital, whereas computer science and coding classes at high school are still often rare, which means that many freshman university students have little experience of using computer software or writing their own code. This lack of experience and hence self-confidence in coding may become a serious hinderance for (successful) data analysis accompanying practical work as students' progress through their academic training, especially in the natural sciences.[1][2]
In this contribution, we present the results of our control group from a freshman course in physical chemistry to illustrate the current problems in traditional teaching in combination with coding aspects and self-determination theory[3] and discuss our approach for a theory of planned behavior (TPB)[4] based interviews with students. Based on this, we will develop a learning unit in the field of spectroscopy to promote students' coding skills and to promote their Self-learning competence. Furthermore, we discuss our approach for a Flipped Classroom to integrate and advance coding skills in MATLAB into a freshman course in physical chemistry education.

Keywords: First-Year Undergraduate; Coding; Higher Education; Flipped Classroom

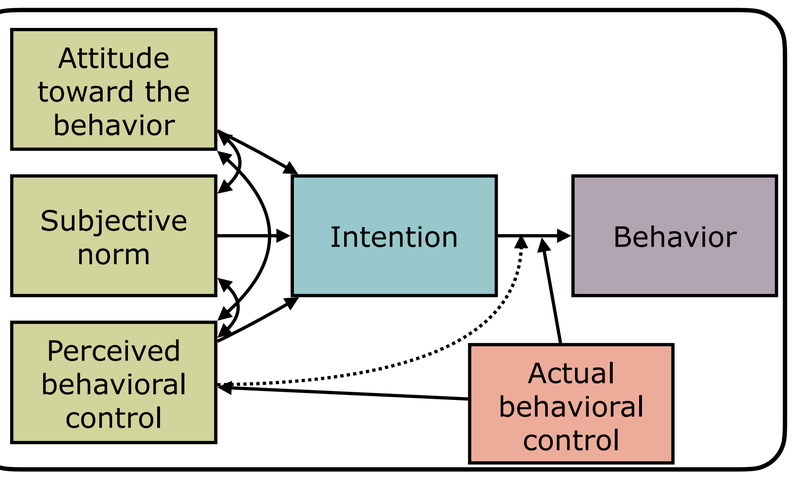
First Control group

- Research based on:
  self-regulated learning, self-determination, self-efficacy on digital learning, attitudes and digital competences

Theory	Dimension	T1	α(T1)
self-regulated learning[5]	goal	2.70	.693
	strategy and time planning	2.12	.812
	self-efficacy	2.77	.795
	self-observation	2.91	.793
	self-evaluation	2.49	.736
	causal attribution	2.94	.880

- No significant changes -> Usual distribution
- Check for scale reliability
- Need of larger control group (N=39)

Interview Study (TPB)



Categories	Description
Properties of digital tools / coding	General description of Coding
Utilisation	Generally for private use or for study
Visualisation	Graphics (analogue or digital)
General conditions	Availability of laptop, Internet, etc.
Attitude	Affinity / Dislike
Social norm	Bandwagon behavior
Behaviour control	Dealing with the fear of programming

Study design

2023

- Question: How to teach Coding in chemistry students?
- Literature research to coding in chemistry[1][2]
- Elaboration of a questionnaire based on educational sciences to Understand students behavior
- Control group in winter term

2024

- Evaluation of the control group
- Can PLAn InC. change students' attitudes towards coding in chemistry?
- TPB interview study on the categorisation of student behavior[4]
- TPB questionnaire

2025

- Elaboration of an intervention based on the results of the TPB questionnaire
- Intervention group in winter term

2026

- Evaluation and Interpretation of the intervention
- Thesis

Comments on Coding

Comment on the following statement:
I find the use of programming within the chemistry curriculum important.

Chemistry consists of conducting a lot of experiments. In order to understand and analyse we need to process the data. Programming is ideal for that.

I don't think it's particularly important because I'm not studying computer science but chemistry.

Unfortunately I can't judge because I'm still new to my studies and don't know anything about computer science.

+			-	N
44	38	20		102

→ neutral students often don't know anything about programming or why to use

Intervention

Flipped classroom

- Activated learning atmosphere
- Exercises & Discussions

Blended Learning

- Videos / Theorical input
- MATLAB tutorials
- Exercises and self tests

Literature:
[1] McCord, R., Jeldes, I. (2019). Engaging non-majors in MATLAB programming through a flipped classroom approach. Computer Science Education. https://doi.org/10.1080/08993408.2019.1599645 [2] Weaver, S. D., Ambrose, G. A., Whelan, R. J. (2022). Activity: Teaching Coding in R through Discipline-Focused Problem- Solving in an Analytical Chemistry Course. J. Chem. Educ., 99, 3068-3073. https://doi.org/10.1021/acs.jchemed.2c00395 [3] Deci, E.L., Ryan, R.M. (1985). *Intrinsic motivation and self-determination in human behavior*. New York: Plenum Press. [4] Ajzen, I. (1985). From intentions to actions: A theory of planned behavior. In J. Kuhl , J. Beckman J (Hrsg.), Action-control: From cognition to behaviour (S.11-39). Berlin Heidelberg New York Tokyo: Springer. [5] Perels, F., Benick, M. und Dörrenbächer-Ulrich, L. (2022). Selbstreguliertes Lernen. In H. Reinders, D. Bergs-Winkels, A. Prochnow, I. Post (Hrsg.*), Empirische Bildungsforschung* (S.713-738). Wiesbaden: Springer.

Quantitative data analysis was performed using IBM Corp. Released 2023 IBM SPSS Statistics for MAC OS, Version 29.0.2.0 (20) Armonk, NY: IBM Corp

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