The design and construction of a PhET-based inquiry learning worksheet to develop understanding of the particle-in-a-box model

Physics Education

PAPER • OPEN ACCESS

The design and construction of a PhET-based inquiry learning worksheet to develop understanding of the particle-in-a-box model

To cite this article: T Bouchée *et al* 2024 *Phys. Educ.* **59** 015031

OPEN ACCESS

PAPER

Phys. Educ. 59 (2024) 015031 (9pp) iopscience.org/ped

The design and construction of a PhET-based inquiry learning worksheet to develop understanding of the particle-in-a-box model

T Bouchée[1,2,*], **L de Putter-Smits**[1], **M Thurlings**[1] and **B Pepin**[1]

[1] Eindhoven School of Education, Eindhoven University of Technology, PO Box 513, 5600 MB, Eindhoven, The Netherlands
[2] Augustinianum, Eindhoven, The Netherlands

E-mail: t.bouchee@tue.nl

Abstract
We report on the design and construction of a worksheet to develop upper secondary school students' understanding of the particle-in-a-box model. We designed a worksheet that guided students' structured-inquiry learning through peer discussion using the PhET simulation 'Quantum Bound States'. The worksheet was improved in three iterative cycles of (re)designing, testing and evaluating, leading to a validated design and tentative design principles. Students' discourse was recorded whilst they were using the worksheet and the PhET simulation in the test phase of each cycle. Analyses of students' discourse informed the redesign of the worksheet for each subsequent cycle, until the design was finalised. The results showed the potential of the simulation to introduce upper secondary school students to the

* Author to whom any correspondence should be addressed.

particle-in-a-box model, provided care is taken to accompany student inquiry with a well-developed worksheet as learning support during the lesson.

Supplementary material for this article is available online

Keywords: quantum physics education, inquiry learning, peer learning, interactive simulation, worksheet design and construction, particle-in-a-box-model

1. Introduction

We describe how we designed a worksheet to introduce Dutch upper secondary students to the commonly used particle-in-a-box model [1] through inquiry learning and peer discussion using the quantum bound states (QBS) simulation from the PhET database [2]. The particle-in-a-box model can be used to describe the behaviour of an electron in a 1D potential well and illustrate how energy levels of the electron are quantised [3].

2. Learning QP with interactive simulations

Interactive simulations were chosen because they can be an effective way to introduce upper secondary students to new quantum physics (QP) concepts and phenomena [4]. Interactive simulations support students by visualizing abstract QP concepts, providing multiple representations, and simplifying complex problems through the consideration of a limited number of variables under idealised conditions [5]. They enable students' inquiry-based learning, promote active participation, transfer responsibility to students to discover new QP knowledge [6], and facilitate peer discussion by providing a common reference point [7].

Inquiry-based learning was chosen since such an approach benefits student engagement and promotes students' understanding of QP by exchanging ideas, articulating conceptual difficulties, and raising new questions [8, 9]. Inquiry-based learning is a student-centred educational approach [10, 11] where students engage in a process of discovering 'new' causal relations by formulating and testing hypotheses through conducting experiments and making observations constructing (for them) new knowledge [12]. Students follow a series of phases based on the scientific inquiry cycle to guide their exploration when interactive simulations are combined with inquiry learning and peer discussion [13, 14].

2.1. Selecting an interactive online simulation

An overview was made of freely-available interactive QP simulations by Google search and snowballing the results. From the over one hundred research-based interactive simulations found online, four addressed the particle-in-a-box model. The 'QBS' simulation was chosen because of: its availability in Dutch, having the most options to freely explore the particle-in-a-box model and that secondary school teachers are familiar and satisfied with PhET simulations [13, 15].

The 'QBS' simulation (figure 1) allows exploring the possible energy levels of an electron in a 1D square potential well as means to understand the particle-in-a-box model. Students can examine how the wave function and probability distribution change with each energy level. The dimension of the potential well can be changed to understand how the width and height of the well affects the possible energy levels of the electron. The user must however understand what is shown on the screen and how it fits or does not fit with their prior physics knowledge. To overcome this latter difficulty we designed a worksheet to structure student thinking.

2.2. Structuring students' inquiries

Student inquiry in small peer groups was chosen to learn QP stimulating self-exploration and peer discussion. *Structured inquiry* from the levels of inquiry formulated by Tamir [16] was selected,

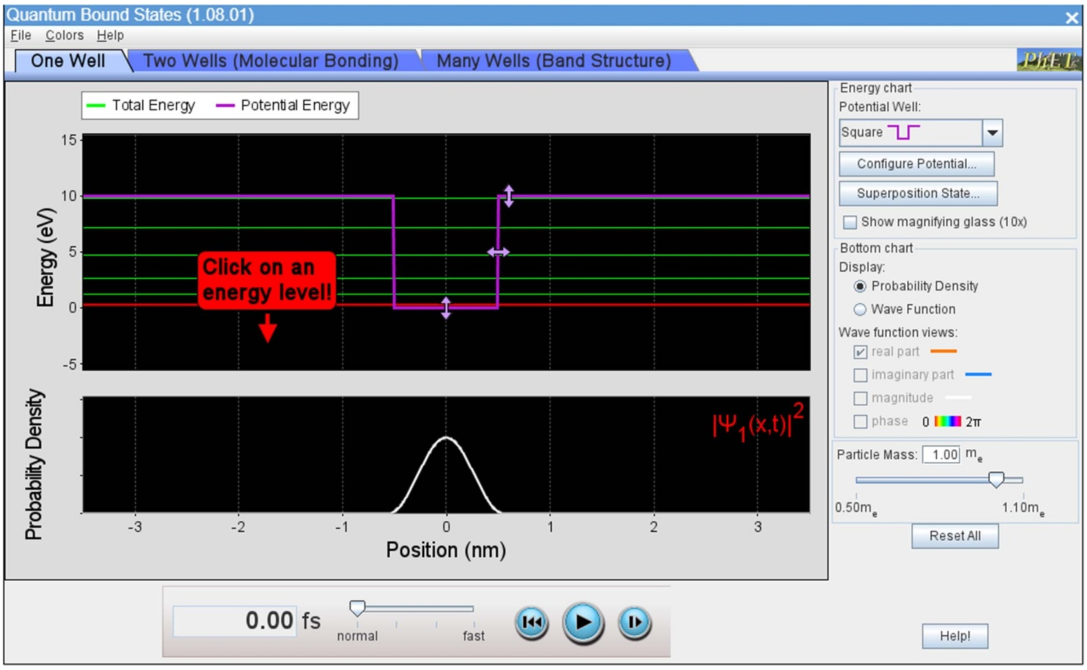

Figure 1. Screenshots of the 'QBS' simulation from the PhET database.

since QP is a new topic in upper secondary physics education and students should then be able to focus on the conceptual foundations of QP by discussing results and formulating new ideas about the new phenomena they encounter. We chose to support students' conceptual understanding in favour of developing students' experimental skills, as conceptual difficulties were expected due to the complexity associated with learning the particle-in-a-box model [17].

3. Method

The worksheet was designed in three micro cycles of (re)design, test, and analysis (see figure 2). The micro-cycles should provide insight into how the lesson around the worksheet should be structured. Two students worked with the designed worksheet for 40 min in the test phase of each micro cycle. The students were asked to think aloud [18] when answering the questions on the worksheet and using the simulation. The students' discourse was audio recorded and transcribed to be able to monitor their developing understanding and identify their reasoning whilst working with the worksheet and simulation.

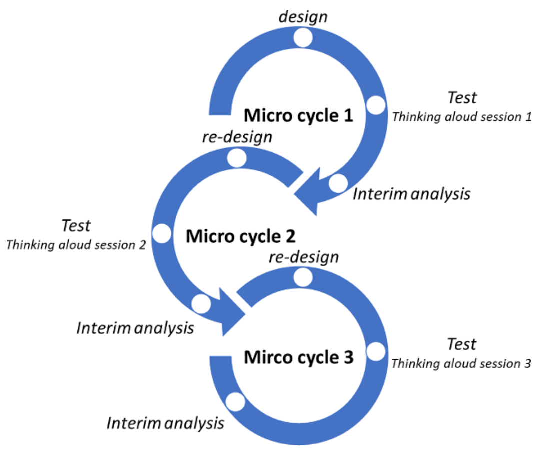

Figure 2. Three micro cycles of design, test, and analysis.

The main researcher moderated each session, asking students to elaborate on their thoughts and summarizing students' answers, checking whether the interpretation was in-line with the thoughts of the students [19]. The researcher would only interfere with a short explanation or a thought-provoking question or remark to help when students were stuck with a specific task.

Six students (aged 17–18—two girls and four boys) from one school in their last year of pre-university education participated in the study. Above-average achieving students were selected to ensure that a lack of physics knowledge and skills would not hinder them. Prior to the study, the students had taken two introductory lessons on QP.

An interim- and post-hoc analysis were conducted on the three thinking aloud sessions. The first consisted of reading the field notes and listening to the audio recordings to uncover redesign steps for the worksheet. The post-hoc analysis was done on the transcriptions to uncover whether students developed an understanding of the QP concepts involved and to identify possible learning difficulties students had. This analysis was used to evaluate design decisions that were made after the interim analysis and to explore how design principles held up in practice. Together these analyses revealed the ways the students used the simulation in addition to the worksheet, revealed any difficulties they had while working with the worksheet, and provided an indication on how a designed lesson using the worksheet would perform in class serving all students.

4. The design of the worksheet

The five phases of Pedaste *et al* inquiry cycle [20] were used to structure the sequence of the worksheet. Questions at the start of the worksheet were on orientation: what concepts do we need before exploring the simulation? Conceptualisation phase questions were on discovering the classical behaviour of a particle in a 1D square potential well. Investigation phase questions were on the behaviour of an electron in a 1D square potential well using the 'QBS' simulation to explore the particle-in-a box model. The conclusion phase focussed on what the student has now learned about the classical and QP case and how both differ. The worksheet design did not incorporate the discussion phase, as we believed it should take place within student groups or even involve the entire class, under teacher guidance.

Five design principles formed the basis to the worksheet (see table 1), where each principle relates to elements the worksheet contained to facilitate the inquiry-based learning of the particle-in-box model using the 'QBS' simulation. The first three principles were based on a literature review and on a context analysis reported on elsewhere [21]. The fourth and fifth design principle were formulated after the post-hoc analysis, and are based on the design decisions made after each micro cycle and the insights obtained from the three thinking-aloud sessions.

4.1. DP1: provide guiding questions

Guiding questions structuring students' inquiry learning, facilitating peer discussion, and avoiding 'learning by doing' or 'trial and error' while using the simulation were included to operationalise this principle [22]. These questions support students' exploration and use of the simulation allowing them to focus on underlying principles governing the simulation's behaviour rather than the required experimental procedures [2, 7] allowing them to test their hypotheses. These questions also served to elicit peer discussion where students discuss together referring to the results shown by the 'QBS' simulation (see [7]).

The students were able to work freely with the interactive simulation during the thinking aloud sessions. The simulation was linked to the text and questions in the worksheet, as was apparent from the student discourse. *'That [the purple line in the simulation] indicates how the electron is able to move within the atom, or no, the molecule* (student 1).*'* The students were trying to shape their ideas on what they saw happening in the simulation. They retrieved existing knowledge to make sense of the workings of the simulation. *'The colour of the dye has something to do with it, because that has something to do with wavelength, or with the amount of energy, do not you think?* (student 1).*'*

Students went back and forth from the questions in the worksheet, to their discussion and kept gesturing at what was visible on the screen. The students were able to discover and formulate that certain energy levels were possible, when asked to explain the different lines in the simulation. *'Well that is of course because there are different energy levels and... if you calculate the kinetic energy then you only have discrete values* (student 5).*'* Discussing the guiding questions together with their peers helped students feed off each other's

Table 1. Design principles for designing a 'QBS' simulation-based inquiry learning worksheet.

Design principle	
DP1	Provide *guiding questions* structuring student inquiries and elicit peer discussions,
DP2	Draw students' attention to *counterintuitive results* comparing classically expected outcomes with results shown in the interactive simulation,
DP3	Include the context of a π*-electron in a molecule* as a real-life application of the particle-in-a-box model,
DP4	Take *students' conceptual difficulties* into account e.g. by adding explanatory text and changing or omitting words that could confuse,
DP5	Use an *analogy of a classical particle* in a square potential to discuss the differences between the classical and QP model.

ideas, attaining the correct interpretation and realise that they uncovered the required answer. For instance, when asked to explain what happens when the 1D square potential increases in length; *'Then the energy levels actually become, … they come closer together and … then automatically more are added* (student 1). *Does the number [of energy levels] remain the same* (student 2)*?' 'No, look if I make it [the potential well] smaller, there will be less* (student 1). *They seem to be compressed. Then more lines are added from above* (student 2). *Yes, they just become, the energy levels become narrower and therefore more are added […] no, there is less difference between the energy levels* (student 1).'

4.2. DP2: draw attention to counterintuitive results

Explicitly drawing students' attention to counterintuitive results should trigger a cognitive conflict seen as a fundamental characteristic for conceptual change [23]. Students need to undergo the process of conceptual change [24] from a deterministic towards a probabilistic worldview [25, 26]. Contrasting students' ideas with the scientifically correct ones using interactive simulations for inquiry-based learning [5] aids to elicit students' prior ideas and challenges them, promoting conceptual change and conceptual understanding [13]. Students were asked in the worksheet to reflect on the differences between classical and QP molecular models based on the information presented by the simulation see [8]). The students interpreted the simulation more and more as each session went on. Towards the end of the session they were able to correctly interpret the simulation and link the workings to the QP model provided. *'Because at the purple line…..ohhh, I get it, because at the purple line he [the electron] is actually out of the well. And this…here the top green line it [the electron] is still in the molecule because then it is in one of those excited states. So you should use the purple line and the ground state. So then you get 10 minus 0.30 which is 9.7 electronvolt* (student 5).'

4.3. DP3: include the 'π-electron in a molecule' as context

We included 'π-electron in a molecule' as a context to explore the QP behaviour of an electron, because it is a real-life application of the particle-in-a-box model [3]. The QP behaviour of a π-electron in a molecule is different from what one would expect classically (e.g. energy quantisation and the different probability distribution). The worksheet started with a brief description of a π-electron and its behaviour in respect to other (σ-) electrons in the molecule. Teachers can struggle to convey the relevance of QP to their students due to a lack of available contexts [21]. The 'π-electron in a molecule' can help provide context, since it can be used to understand the colour of dye molecules and how different dyes can be made by changing the length of the molecule [3], and promote relevance which can motivate students to go through a process of conceptual change.

Students had difficulties understanding the differences between π- and σ- electrons during the thinking aloud sessions. In the first two sessions, students were asked to describe the behaviour of a π-electron in a butene molecule. They had problems understanding that a π-electron could move freely on the molecule. Students held on to molecular models learned in chemistry class to reason about the position and movement of the π-electron. *'With a high energy you have many different places on the molecule where it [the electron] can be… That potential well applies to the entire molecule… […] So you could say, a long molecule at a higher total energy… it [electron] can be here, here, here and here [points to the probability distribution], but when it is lower [the energy level] it [the electron] is only in the middle* (student 3).'

We used the unfamiliar cyanine molecule (a particular dye molecule) to help students understand the difference between π- and σ-electrons for the third session, presuming that this new context made it easier for students to explore the π-electron model as this did not conflict with their understanding of electron configurations learned in their chemistry lessons. It remained difficult for both students in the last session to accept that a π-electron was not bound to an atom in the molecule. *'It [the purple lines] just indicates where those electrons can bond. If I understand correctly, that is the [potential] well around an atom and it [the electron] can bind to that atom* (student 6).'

4.4. DP4: account for conceptual difficulties

We focussed the redesign of the worksheet to account for conceptual difficulties observed during the thinking aloud sessions. These difficulties were that students (a) described wave functions as trajectories of the electron, (b) viewed a potential well as physical object, (c) thought that a change in amplitude meant a change in energy, (d) held on to inappropriate classical (molecular) models, and (e) struggled to activate prior knowledge related to energy diagrams.

During the first thinking aloud session, for instance, a student viewed the potential well as a physical well; *'I just really see it as a well that you have to get out of when you jump* (student 1).' After this session, an explanatory text was added to the worksheet explaining that a potential well is not an actual well, but a space in which the forces acting on the electron bind it to the molecule.

We observed that students had difficulties understanding what 'potential' in potential well meant. In the final version of the worksheet potential well has been replaced by energy well, in line with the textbook students use. Students lacked prior knowledge of energy diagrams as they had difficulties reasoning with negative potential energy. *'Yes, but you cannot potentially have less than what is potent as it were, what it can potentially deliver, so negative [energy] does not seem logical to me* (student 2)'. We therefore decided to exclude questions on negative potential energy from the worksheet not to overcomplicate their inquiries.

4.5. DP5: use a classical analogy

We used a 'tennis-ball-in-a-tube' analogy in the third session, see figure 3, to help students reason about the classical case of a particle in a square potential, to the discuss the differences between the classical and QP model of the object. The first two sessions revealed that students lacked prior knowledge of energy diagrams as they for instance had difficulties expressing how a classical object would behave in a square potential well (e.g. having a continuous energy distribution). The third session showed that this helped students to activate their prior knowledge; *'So you just accelerate the ball, so in principle it can have all possible speeds* (student 6). *Yes indeed […] and it can therefore have all energy levels* (student 5).'

Students 5 and 6 were able to map the 'tennis-ball-in-a-tube' analogy onto the 'π-electron in a molecule' model. *'I think the ball is the electron* (student 5). *Yes, that ball is the electron and I think that the tube is the molecule* (student 6).' We did not find any evidence that the 'tennis-ball-in-a-tube' analogy supported the students to map their understanding from the classical physics domain, triggered by the analogy, onto the abstract QP particle-in-a-box model see [27]). We hypothesise that this mapping from the classical source domain onto the abstract QP target domain was not observed due to time-constraints [28].

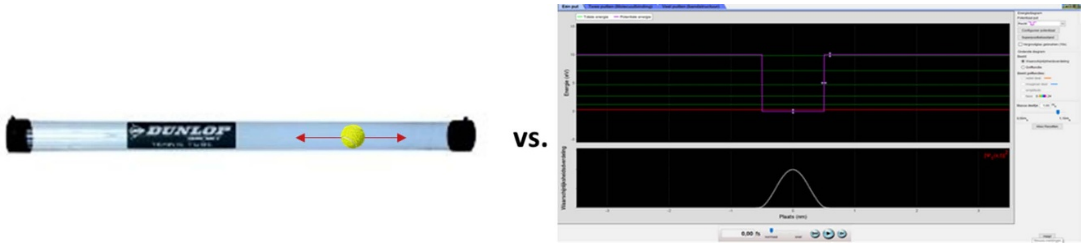

Figure 3. The tennis ball-in-a-tube analogy.

5. Conclusion

This paper examined how a worksheet can be designed for the upper secondary school level combining inquiry-based learning, peer discussion, and the use of the 'QBS' simulation and was improved through three thinking-aloud sessions in which students worked with the worksheet and the simulation. The results suggest the thus designed worksheet has the potential to support upper secondary students' understanding of the particle-in-a-box model.

The worksheet was designed to guide students' structured inquiry-based learning by providing explanatory text and guiding questions. The worksheet supported student learning by providing questions that drew students' attention to counterintuitive results by comparing classical and QP results, helping students challenge their beliefs and monitor their understanding through immediate feedback from the simulation, promoting a process of conceptual change [5]. The context of a 'π -electron in a cyanine molecule' was added to make the abstract particle-in-a-box model more concrete for students by applying it to the real-life context, increasing relevance and student interest [3].

Conceptual difficulties were observed during the three thinking-aloud sessions hindering students' inquiry learning as students had difficulties interpreting the data presented in the simulation correctly [29]. Words that triggered students' conceptual difficulties were changed see [30]. Questions that students found difficult and did not contribute to students' understanding of the main concepts involved were deleted. Explanatory text was added to the worksheet targeting students' conceptual difficulties which in turn was found to support students' conceptual change process [31].

Students held on to the incorrect epistemological assumptions that electrons are bounded to one particular atom in the molecule. The students could not discern between π- and σ- electrons, as they ignored the explanatory text in the worksheets that π-electrons can move freely on the entire molecule. Students might have ignored this information because they assume that scientific content learned in chemistry class is scientifically correct and holds in this new context see [32]. Future research could explore the possible underlying reasons.

We acknowledge the limitations of this study due to the Dutch school context and the small sample size. The Dutch school context is reflected in the physics and chemistry knowledge students have gained per school year. International readers might find their students coming across QP or mentioned chemistry content at a different year or in a different manner. The design principles can be used to rethink and redesign an own worksheet for the own school context even though the principles are tentative. More research is required to further develop these principles. For example, the design principles could be more specific about the types of guiding questions or supports provided to address particular conceptual difficulties. Other analogies or contexts could be used producing comparable results.

Six above-average students participated in this study ensuring students were able to provide valuable feedback on worksheet design before implementation. We saw the worksheet improve as students needed less support learning with the simulation from one session to the next. In the last session, the students were able to answer most questions on the worksheet without assistance. Together, these findings gave us confidence that the final lesson design would hold up in classroom practice. Future research can investigate how the worksheet holds up when used by all students.

Data availability statement

The data cannot be made publicly available upon publication because they contain sensitive personal information. The data that support the findings of this study are available upon reasonable request from the authors.

Acknowledgments

We are thankful to the students for their willingness to participate in this study. Without their time, effort, and openness this paper would not have been possible. This research received funding from the Dutch Ministry of Education, Culture, and Science under the DUDOC program (PhD Grant for teaching and teacher-related studies).

Ethical statement

This research adhered to the ethical guidelines set forth in IOPP's policy. All participants were above the age of 16, and informed consent was acquired from each participant, encompassing both their engagement in the study and the subsequent publication of outcomes.

ORCID iDs

T Bouchée https://orcid.org/0000-0001-7877-7328
L de Putter-Smits https://orcid.org/0000-0003-1507-4785
M Thurlings https://orcid.org/0000-0002-7447-9750
B Pepin https://orcid.org/0000-0001-7804-145X

Received 15 August 2023, in final form 8 November 2023
Accepted for publication 4 December 2023
https://doi.org/10.1088/1361-6552/ad11f8

References

[1] Stadermann H K E, van den Berg E and Goedhart M J 2019 Analysis of secondary school quantum physics curricula of 15 different countries: different perspectives on a challenging topic *Phys. Rev. Phys. Educ. Res.* **15** 010130
[2] McKagan S B, Perkins K K, Dubson M, Malley C, Reid S, LeMaster R and Wieman C E 2008 Developing and researching PhET simulations for teaching quantum mechanics *Am. J. Phys.* **76** 406–17
[3] Hoekzema D, van den Berg E, Schooten G and van Dijk L 2007 The particle/wave-in-a-box model in Dutch secondary schools *Phys. Educ.* **42** 391
[4] Bouchée T, de Putter-Smits L, Thurlings M and Pepin B 2022 Towards a better understanding of conceptual difficulties in introductory quantum physics courses *Stud. Sci. Educ.* **58** 183–202
[5] Smetana L K and Bell R L 2012 Computer simulations to support science instruction and learning: a critical review of the literature *Int. J. Sci. Educ.* **34** 1337–70
[6] De Jong T and Joolingen W R 1998 Scientific discovery learning with computer simulations of conceptual domains *Rev. Educ. Res.* **68** 179–201
[7] Rehn D A, Moore E B, Podolefsky N S and Finkelstein N D 2013 Tools for high-tech tool use: a framework and heuristics for using interactive simulations *J. Teach. Learn. Technol.* **2** 31–55
[8] Bungum B, Bøe M V and Henriksen E K 2018 Quantum talk: how small-group discussions may enhance students' understanding in quantum physics *Sci. Educ.* **102** 856–77
[9] Deslauriers L and Wieman C 2011 Learning and retention of quantum concepts with different teaching methods *Phys. Rev. Spec. Top.-Phys. Educ. Res.* **7** 010101
[10] Martin-Hansen L 2002 Defining inquiry: exploring the many types of inquiry in the science classroom *Sci. Teach.* **69** 34–37
[11] Keselman A 2003 Supporting inquiry learning by promoting normative understanding of multivariable causality *J. Res. Sci. Teach.* **40** 898–921
[12] Pedaste M, Mäeots M, Leijen Ä and Sarapuu T 2012 Improving students' inquiry skills through reflection and self-regulation scaffolds *Technol. Instruct. Cogn. Learn.* **9** 81–95
[13] Banda H J and Nzabahimana J 2021 Effect of integrating physics education technology simulations on students' conceptual understanding in physics: a review of

literature *Phys. Rev. Phys. Educ. Res.* **17** 023108
[14] Rodriguez L V, van der Veen J T, Anjewierden A, van den Berg E and De Jong T 2020 Designing inquiry-based learning environments for quantum physics education in secondary schools *Phys. Educ.* **55** 065026
[15] Perkins K K, Moore E B and Chasteen S V 2014 Examining the use of PhET interactive simulations in US college and high school classrooms *Proc. 2014 Physics Education Research Conf.* pp 207–10
[16] Tamir P 1991 Practical science: the role and reality of practical work in school science eds B E Woolnough (Open University Press) pp 13–20
[17] Krijtenburg-Lewerissa K, Pol H J, Brinkman A and van Joolingen W R 2020 Secondary school students' misunderstandings of potential wells and tunnelling *Phys. Rev. Phys. Educ. Res.* **16** 010132
[18] Charters E 2003 The use of think-aloud methods in qualitative research an introduction to think-aloud methods *Brock Educ.* A **12** 68–82
[19] Miles M B, Huberman A M and Saldana J 2014 *Qualitative Data Analysis* (SAGE Publications)
[20] Pedaste M, Mäeots M, Siiman L A, De Jong T, Van Riesen S A N, Kamp E T, Manoli C C, Zacharia Z C and Tsourlidaki E 2015 Phases of inquiry-based learning: definitions and the inquiry cycle *Educ. Res. Rev.* **14** 47–61
[21] Bouchée T, Thurlings M, de Putter-smits L and Pepin B 2023 Investigating teachers' and students' experiences of quantum physics lessons: opportunities and challenges *Res. Sci. Technol. Educ.* **41** 777–99
[22] Haagen-Schützenhöfer C and Hopf M 2020 Design-based research as a model for systematic curriculum development: the example of a curriculum for introductory optics *Phys. Rev. Phys. Educ. Res.* **16** 020152
[23] Potvin P *et al* 2020 Models of conceptual change in science learning: establishing an exhaustive inventory based on support given by articles published in major journals *Stud. Sci. Educ.* **56** 157–211
[24] Vosniadou S, Ioannides C, Dimitrakopoulou A and Papademetriou E 2001 Designing learning environments to promote conceptual change in science *Learn. Instr.* **11** 381–419
[25] Bøe M V, Henriksen E K and Angell C 2018 Actual versus implied physics students: how students from traditional physics classrooms related to an innovative approach to quantum physics *Sci. Educ.* **102** 649–67
[26] Bungum B, Henriksen E K, Angell C, Tellefsen C W and Bøe M V 2015 ReleQuant: improving teaching and learning in quantum physics through educational design research *Nord. Stud. Sci. Educ.* **11** 153–68
[27] Kersting M and Steier R 2018 Understanding curved spacetime: the role of the rubber sheet analogy in learning general relativity *Sci. Educ.* **27** 593–623
[28] Niebert K, Marsch S and Treagust D F 2012 Understanding needs embodiment: a theory-guided reanalysis of the role of metaphors and analogies in understanding science *Sci. Educ.* **96** 849–77
[29] De Jong T, Van Joolingen W R, Swaak J, Veermans K, Limbach R, King S and Gureghian D 1998 Self-directed learning in simulation-based discovery environments *J. Comput. Assist. Learn.* **14** 235–46
[30] Brookes D T and Etkina E 2007 Using conceptual metaphor and functional grammar to explore how language used in physics affects student learning *Phys. Rev. Spec. Top.- Phys. Educ. Res.* **3** 010105
[31] Chi M T H 2008 Three types of conceptual change: belief revision, mental model transformation, and categorical shift *International Handbook of Research on Conceptual Change* ed S Vosniadou (Routledge) pp 61–82
[32] Kalkanis G, Hadzidaki P and Stavrou D 2003 An instructional model for a radical conceptual change towards quantum mechanics concepts *Sci. Educ.* **87** 257–80