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Chemical Education Research

High School Students Experimenting with Computational Chemistry: Design-Based Research on and through the "Comp-Chem-Lab"

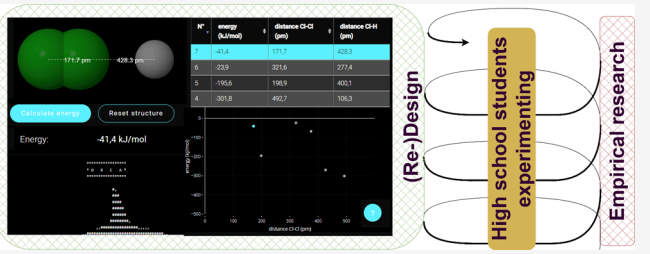
Benjamin Pölloth*

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ABSTRACT: Despite the profound impact of Computational Chemistry (CC) on chemical research and understanding, it plays a negligible role in high school chemistry curricula. Integrating CC into high school education could enable students to engage in authentic science simulations and deepen their understanding of energy. To enable high school students to use CC, a freely accessible online learning environment, the Comp-Chem-Lab (www.comp-chem-lab.de/en), was developed based on qualitative empirical data from 80 German high school students in a design-based research approach. With this environment and the adaptive feedback implemented, most students were able to successfully use CC to determine the activation energy and released energy of a chemical reaction. A common progression of problem-solving strategies is for students to begin with trial and error but later to explore the relationship between chemical structure and energy more strategically based on their CC results. After searching for a "zero" energy structure, most students eventually activate the idea of energy minimization and successfully transfer it to another reaction step. Overall, the research highlights the potential of CC for enhancing high school and introductory college chemistry education but also emphasizes the need for further educational research to fully realize this potential.



KEYWORDS: *Chemical Education Research, High School, Computational Chemistry, General Chemistry, Web-Based Learning, Inquiry-Based Learning, Covalent Bonding, Free Radicals*

For centuries, laboratory experiments were the primary, if not the only, way to gain new knowledge in chemistry. In recent decades, the advent of computational chemistry (CC) has provided a second, readily accessible way to gain insight into chemical processes. Houk and Liu state: "Computational chemistry has progressed from a rarity to become a full partner with experiment in the investigation of organic and biochemical structures and reactions."[1]

Therefore, one would expect CC to play a central role in chemistry education. In fact, it could allow students to conduct inquiry-based experiments on the energy of the chemical structures and reactions. This is an area in which many students lack well-connected conceptual knowledge.[2−4] Yet in many countries, including Germany, CC is mentioned neither in high school curricula[5] nor in university courses for teacher's degree students.[6,7] The limited adoption of CC in education may be attributed to the complexity of current technical implementations, which are often too advanced for high school students and insufficiently tailored to the specific needs of high school curricula.

In this study, design-based research (DBR) was used to develop an online learning environment that allows high school students to investigate a model reaction using CC. The resulting Web site is called "Comp-Chem Lab" (CCL) and can be used free of charge at www.comp-chem-lab.de/en. Although this site was developed for a German high school setting, it may also be a helpful tool for discussing energetic aspects of chemical reactions or reaction coordinate diagrams in the context of a first-year general chemistry course.

THEORETICAL BACKGROUND

Computational Chemistry

The common core of all CC methods is to find the system with the lowest energy. A broad variety of methods is used to reach this goal.[8] Some are based on Newtonian mechanics (e.g., molecular mechanics or molecular dynamics); others are based on quantum chemical models. Quantum chemical (QC) methods compute approximate solutions of the Schrödinger equation, with which the energy of a chemical structure can be calculated.[9] The most common QC methods, e.g., *ab initio*

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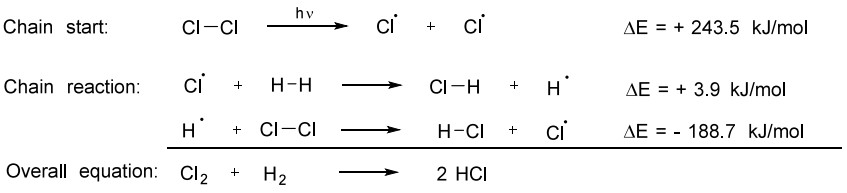


Figure 1. Reaction scheme of the radical chain reaction of hydrogen and chlorine.[16]

methods or density functional theory (DFT), divide the energy of a molecule, in very simplified terms, into the kinetic energy of the electrons and the negative and positive potential energy. The negative potential is caused by the attractive forces between atomic nuclei and electrons, while the positive potential is due to the repulsive forces between electrons. A comprehensive introduction to CC and QC can be found elsewhere.[8,9]

Simulations as a Tool for Scientific Inquiry and Learning

Research shows that the use of computer technology and simulations can enhance students' learning achievements.[10] Student scientific inquiry skills are especially fostered when simulations provide additional feedback, as suggested in a meta-study by D'Angelo et al.[10] It should be noted, however, that the term "simulation" is often used indistinctly in the educational context. Winsberg defines: "A computer simulation is a program that is run on a computer and that uses step-by-step methods to explore the approximate behavior of a mathematical model. Usually this is a model of a realworld system."[11] Scientific simulations should be clearly distinguished from interactive animations that are not based on scientific models and are not authentic tools for scientific inquiry.[12] From this perspective, QC calculations are "real" scientific digital simulations based on quantum mechanical models.

The gap between chemistry research and high school education could be bridged by implementing CC in chemistry classrooms. CC could complement laboratory experiments in inquiry-based chemistry learning. In fact, a number of studies have shown that combining real and virtual experiments improves conceptual understanding.[13] From a learning theory perspective, this can be rationalized as the different representations trigger different learning mechanisms.[14] Also in chemistry research, the most reliable and insightful use of CC is in combination with physical experiments. Therefore, the use of CC in this study is examined in the context of a model reaction that can be performed experimentally.

The Reaction of Chlorine and Hydrogen as a Model Reaction

A common model reaction is the reaction of molecular hydrogen and chlorine to form gaseous hydrogen chloride.[15] The reaction mechanism can be described best by the radical chain reaction scheme shown in Figure 1.[16] QC research suggests that atom transfer in chain reactions occurs in a collinear fashion.[15]

We chose the reaction of hydrogen and chlorine as a model context because

(1) it has molecular reactants and products, making it easy to handle with CC;
(2) it involves a maximum of three atoms per reaction step, which simplifies both students' reasoning and CC calculations;
(3) it can be understood at high school level; and
(4) it can be demonstrated in school experiments (Figure 2).[17]

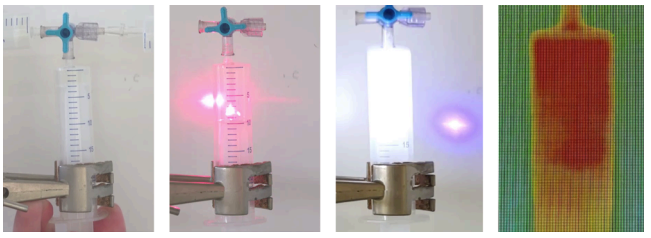


Figure 2. Screenshots of the experiment video. (1) A 1:1 mixture of chlorine and hydrogen gas in a syringe; (2) the mixture is irradiated with red light, no reaction occurs; (3) after irradiation with blue light, an explosive reaction occurs; (4) a thermal imager shows that heat is produced.[17]

When the reaction mixture is irradiated with light of sufficient energy to break the chlorine-chlorine bond, a highly exothermic chain reaction takes place.[16] Hence, in this reaction, the core ideas of energy, chemical structure, and reaction are closely intertwined. Understanding these relations is a major challenge in learning chemistry.

Student Understanding of Energy in Chemical Reactions

Conceptual student understanding of energy is often low and linked insufficiently to other core concepts.[18,19] Alternative ideas on energetic phenomena like exothermic bond breaking,[20] or equation of energy transfer and heat flow[21] are common. Learners find it particularly difficult to explain macroscopic energy changes productively on a submicroscopic level.[22,23] Consequently, students seldom refer to energetic aspects in mechanistic reasoning,[24] in rationalizing chemical bonding,[25] or when explaining the driving force of reactions.[26]

In preparation for this study, we wanted to explore which cognitive resources high school students activate to rationalize energetic aspects of the model reaction of chlorine and hydrogen (Figure 2).[2,27] This investigation was done in the context of the high school system of Baden-Württemberg.[28] The curriculum follows a traditional approach focusing on bond types.[25] Most high school students from this background explained activation energy using technical terms rather than discussing bond breaking. Only one group of 16 referred directly to newly formed bonds to explain the released energy. Most students relied on the octet rule to explain why a reaction occurred.[29,30] Many students used reaction coordinate diagrams (RCDs) in their explanation but mostly interpreted them on a macroscopic and temporal scale rather than in terms of structure and energy.[31] Overall, we found that students' struggles with the role of energy in chemistry became particularly evident in their explanation of the chosen model reaction.

One explanation for students' difficulties may be that energy is difficult to study and quantify experimentally.[32,33] Hence, the implementation of CC in high school chemistry could improve students' understanding of the relationships among energy, structure, and reactivity.

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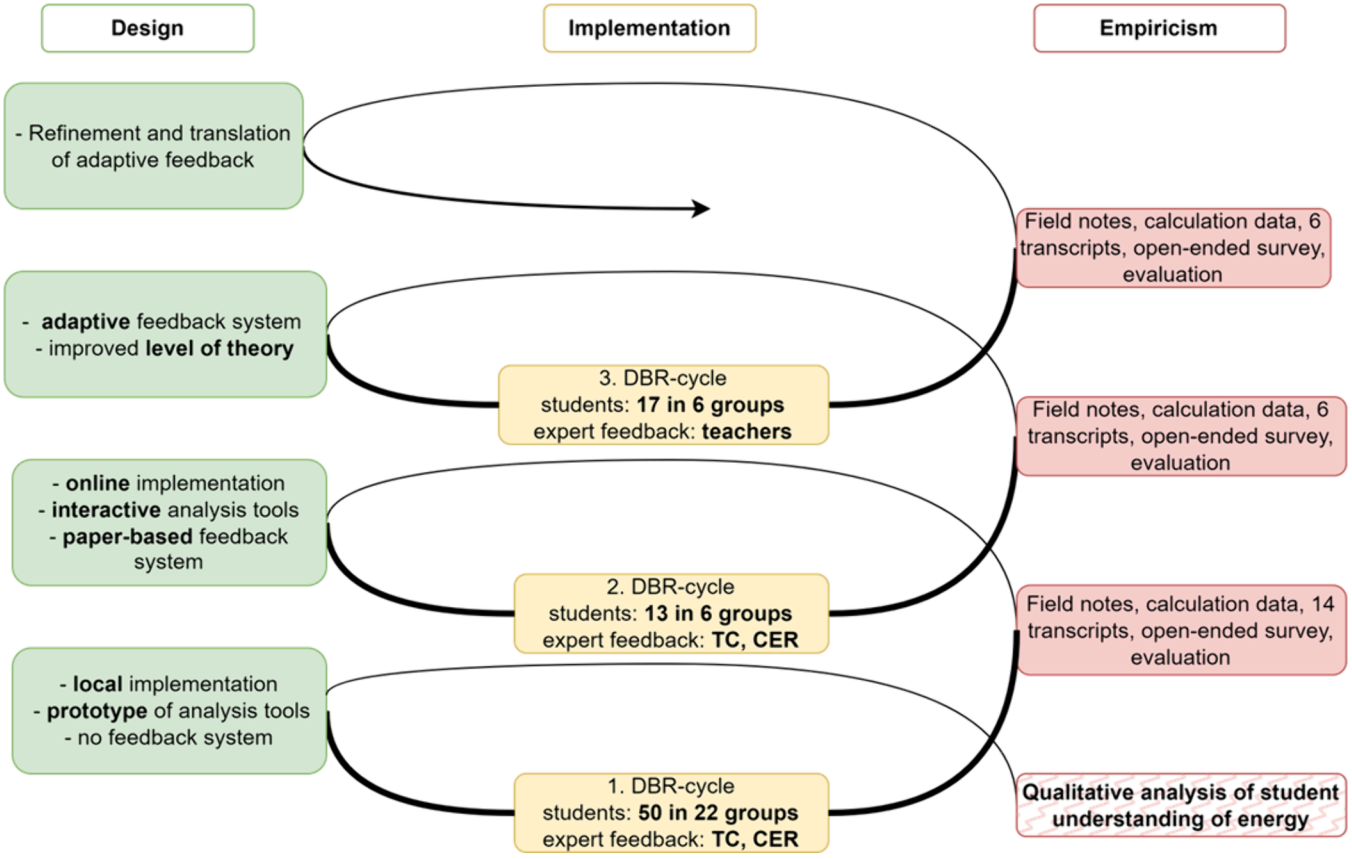


Figure 3. Overview of the DBR process showing the evolution of the design, implementation, and empirical methods used in each cycle.

Implementation of CC in Chemistry Teaching

Nearly 30 years ago, the *Journal of Chemical Education* titled "Computational Chemistry for the Masses"[34] and described how CC is integrated into undergraduate chemistry education.[34,35] Since then, "computational chemistry literacy" has become one of the goals of many undergraduate chemistry curricula.[36,37] Therefore, a variety of teaching methods and tools for CC are presented in chemistry education literature.

Specific CC learning environments were developed for the students. *eChem* is an interactive notebook which interactively guides students through the fundamentals of theoretical and computational chemistry.[38] ChemCompute is a Web site that allows undergraduates to use computational chemistry software.[39]

However, in contrast to the evolving integration of CC into university chemistry, CC has not had a profound impact on high school chemistry yet.[7] Many interactive animations of chemical reactions commonly used in high school are not grounded at all on scientific simulation.[40,41] Several interventions used simulations based on Newtonian mechanics, e.g., on dynamic molecular simulations,[42,43] or on molecular mechanics mainly using Avogadro.[7,44,45] Avogadro uses force field methods (FFM) to optimize structures that do not allow the study of bond breaking and formation.[9] QC methods are better suited to this purpose. Hrubeš et al.[6] recently studied the use of QC with high-achieving high school students giving lectures on the basics of QC and using Gaussian to solve problems, including a scan of bond lengths in the hydrogen molecule. Statistical analysis showed an increase in student confidence in chemistry. As a limitation, Hrube et al. note that their approach requires instructors who are familiar with QC, which may not be the case for most teachers.

Tuvi-Arad[36] described several teaching and learning challenges for integrating CC into the undergraduate curriculum, which may be even more pronounced for high schools. These challenges include

- infrastructure (software and hardware availability),
- students' technical training (use of complex CC interfaces),
- class time constraints and theoretical background,
- instructors' technological, pedagogical, and scientific knowledge of CC,
- and instructors' self-efficacy regarding their ability to integrate CC into their teaching.

To address these challenges, it seems desirable to develop an implementation of CC that does not require specific hardware or software and can be used without specific knowledge of CC but at the same time allows all high school students to explore chemical concepts with CC in a flexible way. This project uses design-based research to achieve this goal.

Design-Based Research

The core idea of DBR is to merge empirical research on learning with the systematic engineering of educational interventions in an authentic context.[46] DBR studies are interventionist, theory-based, and reflective.[47] A key feature of DBR is its iterative nature. A theory-driven prototype of an educational intervention is adapted to learners' needs through flexible design revisions based on empirical observations.[47] One DBR-iteration is characterized by (1) (re)design of instructional tools, (2) the test in a real-world learning environment, (3) the empirical

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evaluation of the learning process, and (4) a reflection on how to further improve the design.[48] However, it should be emphasized that the goal of DBR is not only to engineer a product but also to develop learning theories.[47] Thus, a DBR process can involve research *for* (e.g., analysis of existing interventions, empirical studies of learner prerequisites), *on* (development of the educational tool), and *through* the intervention (gaining insights into learning processes).[49]

RESEARCH GOAL

The overall goal of this project is to investigate how far high school students can use CC experiments to actively explore the energetic aspects of a chemical reaction. In a qualitative empirical study *for the intervention* we investigated the cognitive resources activated by secondary school students to explain energetic aspects of the reaction of hydrogen and chlorine as briefly summarized above.[2] Based on these findings, this project focused on research questions *on* and *through* the intervention:

1. What design features should an online platform include to enable high school students to explore bond lengths and simple chemical reactions using CC?
2. What strategies do high school students employ when using CC to investigate bond lengths and the energetics of simple chemical reactions?

METHODS

Sample

All high school students in the sample were enrolled in grades 11−13 of an academic track high school in the German state of Baden-Wuerttemberg. Details of the curriculum are described in previously published articles.[2,30]

The intervention of the CCL took place in the context of an out-of-school laboratory. The laboratory visit was mandatory for school classes, but study participation was voluntary.

Three major DBR iterations with a total of 80 high school students were performed (Figure 3):

- Cycle 1:50 high school students in 22 groups, feedback by experts in Theoretical Chemistry (TC) and in Chemistry Education Research (CER)
- Cycle 2:13 high school students in 6 groups, feedback by experts in TC and CER
- Cycle 3:17 high school students in 6 groups, practitioner feedback through implementation in four teacher training workshops

Informed consent for the use of the data for scientific research and publication was obtained from all students and, in the case of minors, their parents. The study design was approved by the Faculty of Economics and Social Sciences Ethics Committee (2022−04−06) of the University of Tübingen.

Data Collection and Processing

All students worked in focus groups of two or three. After watching the experiment video (Figure 2), they were asked to explain the observations by solving the four tasks listed in Box 1. The first two tasks were motivated by explaining why blue light is needed; tasks three and four by explaining why the reaction is exothermic. The CCL also included a fifth expert task using a three-dimensional potential energy surface. The tasks in cycles 1 and 2 were paper-based, while in cycle 3 they were embedded directly into the home page. The wording of the problems differed slightly between the cycles. Students worked with the CCL for 30 to 60 min to complete the tasks. Students were encouraged to work independently as much as possible. When questions arose, students were first encouraged to use the embedded feedback system (in cycles 2 and 3). Whenever additional support was needed, teaching assistants (TAs) were available to help the students.

Box 1. Tasks to Be Solved by Students in CCL Experiments

1. What is the distance between two chlorine atoms in a chlorine molecule (Cl_2)?
2. How much energy is needed to split a chlorine molecule in two chlorine atoms?
   The reaction involves the following reaction step: Cl−Cl + H· → Cl· + H−Cl
3. Determine how much energy is released in the given reaction step.
4. Determine the activation energy for the given reaction step.

The following empirical data was collected:

- **Field notes:** The author observed all focus groups and took field notes. Due to the exploratory nature of this study, no specific observation guide was followed. The field notes comprise reports on bugs, student difficulties, and general observations.
- **Transcripts of focus groups:** 26 of the 34 focus groups agreed to have their consultations and screens recorded while working with the CCL. Auditive material relevant to the work with the CCL was transcribed. Unrelated material was not transcribed to reduce the amount of data.
- **Calculation data:** All CC calculation data (chosen structure, computed energy, in cycle 3: given adaptive feedback) was saved and transferred into Excel tables.
- **Open-ended Survey:** Students were asked to take notes on any bugs, ambiguities or difficulties with the CCL. After their work, students answered an open-ended survey including questions on possible improvements of the software and the potential they saw in the CCL (see SI).
- **Evaluation data:** At the end of their day at the out-of-school laboratory, students rated the activities of their visit, including three laboratory experiments and working with the CCL, on a five-point Likert scale. Full details and mean scores are documented in the SI.

The study was conducted in German. All quotations in the manuscript were translated as literally as possible; the original German statements are reported in the SI. The number in the group name indicates the DBR cycle.

Data Analysis

For the data-driven control and refinement of the design features, field notes, transcripts, and responses to the open-ended survey were combined into a single MaxQDA file. The combined data were analyzed employing qualitative content analysis according to Kuckartz[50] and coded into three main categories: (1) suggestions for improvement, (2) praise for the CCL, (3) problems and challenges. Subcategories were formed inductively (see SI). Coding was conducted by BP. Intercoder reliability was ensured by recoding the data by an independent TA using a consensus approach.

In a second step, students' problem-solving strategies were analyzed based on the transcripts and the calculation data. Only data from students in cycles 2 and 3 were used. Data from cycle 1

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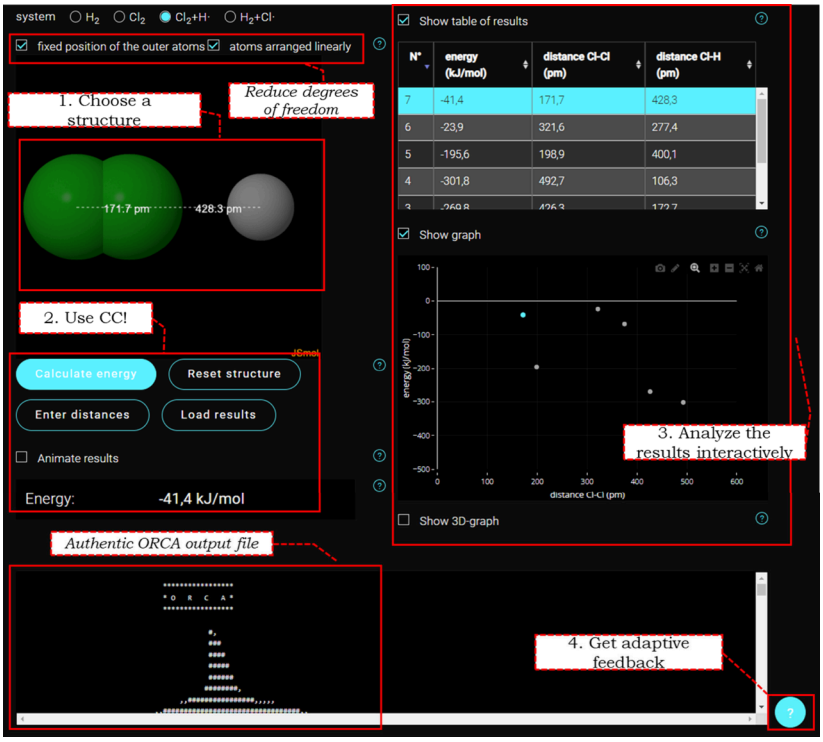


Figure 4. Screenshot of the final version of the CCL highlighting the developed features. The web site is accessible free of charge at www.comp-chem-lab.de/en/h2cl2.

were excluded due to changes made in both the task and the CCL itself. In contrast, cycles 2 and 3 differed only in the CC method used and in the provision of adaptive feedback (paper-based in cycle 2 vs digital in cycle 3). For the qualitative analysis, these minor deviations were not considered significant. The 12 remaining transcripts were combined with the calculation data. The problem-solving approaches were identified through a qualitative content analysis. BP inductively derived categories of solving strategies. Based on these categories, four transcripts were recoded by a TA. Some categories were found to not be selective enough and were merged (e.g., "trying out" and "targeted trying out"). Any differences between the coders were discussed, and consensus was reached through discussion.

The quantitative evaluation data were intended to be analyzed in only a descriptive manner. The small and nonrepresentative sample size does not allow for any further quantitative comparison. The full quantitative data can be found in the SI.

DESIGN FEATURES OF AN ONLINE CC PLATFORM

This section describes the development of a platform that allows high school students to work with authentic CC. Figure 4 presents an overview of its design features in their final form.

Identification of an Appropriate Level of Quantum Chemistry

One core idea of CCL is the use of authentic CC methods. As students are not expected to have prior knowledge of CC, an appropriate level of theory was preselected (see SI for detailed information). If overly simplistic CC methods (e.g., Hartree–Fock) are used, the resulting bond dissociation energies (BDE) deviate significantly from the experimental values. With the chosen level of theory a quite accurate BDE of −247 kJ/mol (experimental BDE: −239.7 kJ/mol)[51] is found. It allows to discuss why red light with an associated energy of 167 kJ/mol does not allow to break the chlorine-chlorine bond but blue light (corresponding to 293 kJ/mol) does.[52]

On the other hand, some uncertainty is inherent in model-based simulations. For instance, the resulting bond dissociation curves in the CCL are not flawless. They exhibit disruptions at certain distances, as observed in the data. Students noted these irregularities:

2: What are these disruptions here? 1: I'm not quite sure yet. (3F)

Processing of the Computed Values

Analyzing CC output files exceeds the knowledge of most high school students. Therefore, a semiautomatic analysis has been implemented: In the CCL, the energy of atoms in "infinite distance" from each other, i.e. isolated atoms, is calculated as the reference energy (Figure 5). The reference energy value is subtracted from the single point energy of the chosen structure, and the resulting value is converted to kJ/mol (eq 1). This energy can be interpreted as the total interaction energy between the atoms.

$$E_{Displayed} = (E_{ChosenStructure} - E_{VeryDistantAtoms}) \cdot 2625.5\ \text{kJ/mol} \quad (1)$$

In addition to these energy values, the complete output data from the ORCA computation are displayed in the CCL. The goal is to enhance the authenticity of the learning environment. In fact, many student groups reviewed the output files and expressed interest in them:

1: Well, I think it really has to do a lot of math. 2: What do they have to calculate? 1: Yes, it has to... Down there... Look (scrolls through the ORCA output). 2: For God's sake, but that is not for us. (laughing, keeps on scrolling) (3A)

Selection of Chemical Structures

Each step of the reaction of chlorine and hydrogen (Figure 1) can be investigated in the CCL. The atoms involved in a specific

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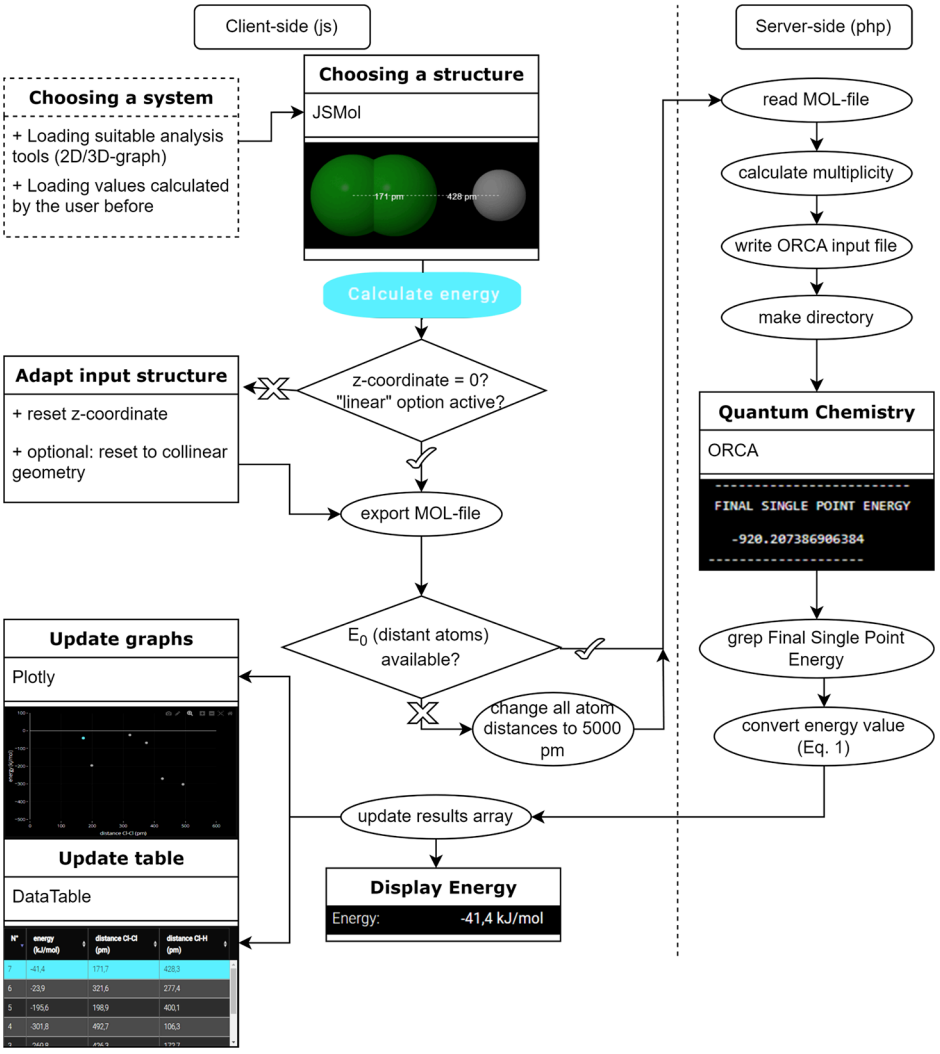


Figure 5. Flowchart of the working process of the CCL. The chosen structure of the user is translated into an MOL file. After several corrections (details in the SI) the energy is computed by ORCA on an external server, and the analysis tools are updated.

step can be moved by drag-and-drop using JSMol.[53] Atoms are currently visualized as simple spheres with the van der Waals radii of the respective elements. Bonds are not represented. Expert feedback on the very simple representation of atoms were contradictory. However, after testing different visualizations, we chose to stick to the simplest model to keep the cognitive load as small as possible. No student in the sample had problems interpreting the spheres as atoms. In fact, representing bond formation and dissociation is challenging as a certain cutoff distance for chemical bonds must be defined. Thus, the represented bonds would "suddenly" disappear, contradicting the idea of a continuous spectrum of electrostatic interactions.[3]

A common observation was that students became confused when choosing a structure because they unintentionally rotated the entire molecule in 3D space instead of changing the position of just one atom. To avoid this problem, the z-coordinate of the (2D) structure is set to zero before each calculation.

Analysis of Energy Values

The crucial step in CC research is interpretation of the resulting energy values in the context of the chemical question. Students in the CCL can perform these analyses by using the isolated values, sortable tables, and interactive graphs. The observation data show that students used the graphs and table extensively.

3: Look, we have this graph here; perhaps we could try out different things. [...]

1: Maybe the distance keeps on increasing the distance. Start very small and then keep going. Then we already have an idea.

[the group proceeds from two- to three-atomic systems]

2: We can create a graph again, that means, calculate different values and then

3: Then we can guess again which point we should look for or what?

1: We can just move it [the atom] a little bit. (1J)

Because of the important role of these tools, their interactivity has been further increased during the DBR process: Clicking on a specific point in the graph displays the corresponding structure and data entry in the table and vice versa. Students used these options frequently to connect energy and structural level.

Reducing Degrees of Freedom

One challenge in the investigation of chemical reactions with CC is the quickly increasing number of geometric degrees of freedom (DOF). Two-atomic molecules have only one DOF (the bond distance), and energy can be plotted as a function of the bond distance. For three-atom molecules, this is possible only in a four-dimensional graph. To simplify the analysis, CCL offers two options to reduce the number of DOFs. One option

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forces the three atoms into a collinear arrangement (Figure 6, bottom).[15] In a second option, the coordinates of the two outer

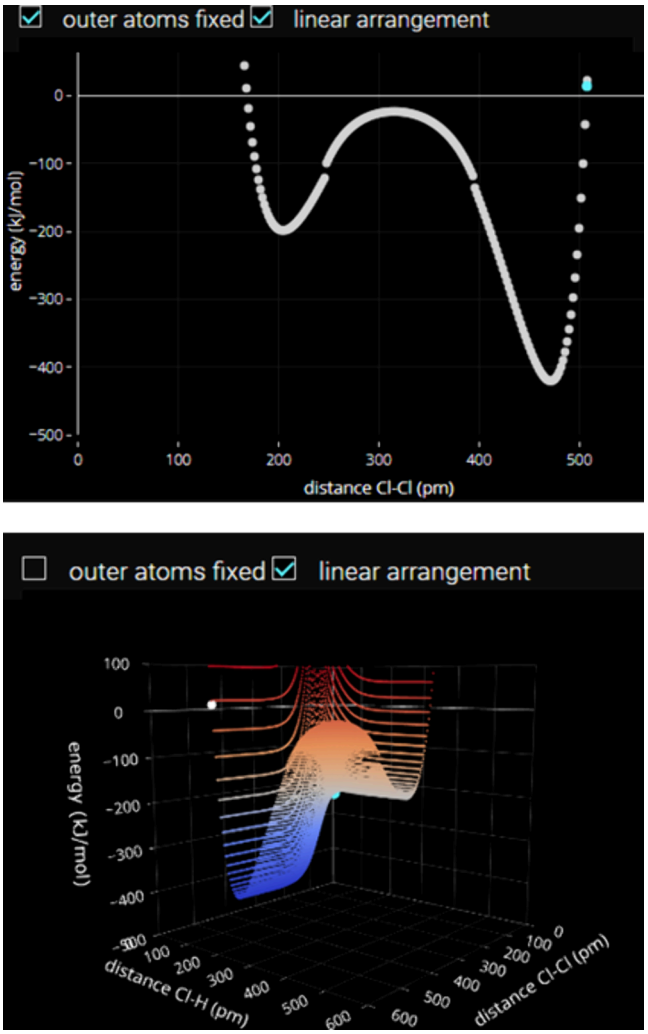


Figure 6. Analysis of the reaction of chlorine and hydrogen with different degrees of freedom: (top) linear alignment with frozen outer atoms: analysis of the potential energy curve in a two-dimensional graph; (bottom) linear alignment with moving outer atoms: analysis of the potential energy surface in a three-dimensional graph; the fully unrestricted setting cannot be shown because it requires a four-dimensional graph.

atoms are frozen, resulting in only two DOF. The reaction can then be modeled by moving the central atom and analyzed in a 2D distance-energy diagram (Figure 6, top).

These diagrams reminded many students of reaction coordinate diagrams. Activating these resources helped students interpret their results:

3: Ah, this is the activation energy (points to the first minimum and peak). This is nothing more than an exothermic reaction. This is the graph we had. And the energy level (points to final point) is lower, which is why the reaction reacts. (3E)

Furthermore, the CCL allows more advanced students to explore the 3D potential energy surface for the reaction steps by providing precalculated energy values. Some students discussed different reaction pathways and identified the lowest energy path:

Instead of going this way, up here and then down again [points to reaction path from two-dimensional calculation], we go this way and then down here [points to path of minimum energy]. Because that looks like less. That means the point we are looking for is somewhere here [points to the correct transition state]. (3F)

Adaptive Feedback

The most common request from students in the survey was to implement a more detailed feedback system. Therefore, adaptive rule-based feedback was integrated into the CCL. In cycle 1, TAs verbally helped students in solving the problems. The transcripts of these interventions were analyzed to identify students' struggles and to determine helpful feedback. In cycle 2, students received a printed version of the hints. Based on the observations in cycle 2 an adaptive feedback system was developed and tested in cycle 3.

The feedback system allows students to enter their answers for the specific task. By checking the answers as well as the calculations performed, we provide adaptive feedback is provided. Additionally, students can request help by clicking on a special button. The system analyzes the structures that the student has explored and gradually provides assistance. Many students praised the usefulness of the adaptive feedback system:

I think the hints are great. (group 3A)

[Particularly helpful in the software were] the hints, explanations, and the presentation of the results (group 3D)

Developing an adaptive feedback system manually is tedious. In its current form, the adaptive feedback system already covers nearly a hundred *if conditions*. New technologies, such as generative AI, could simplify and improve the delivery of such feedback systems.[54,55]

Student Rating of the CCL

Students were asked to rate a series of given statements on the CCL using Likert-type scales (see SI for the questionnaire). 62% of the students (rather) agreed that they learned many new things about chemistry, and 79% (rather) agreed that they got insights into methods of chemical research. For example, one student highlighted:

[My take-home message is] Chemistry is not only in the lab but also digital.

Several students mentioned the CC experiments as the highlight of their out-of-school lab visit. 55% agreed that working with the CC experiments was fun, while 23% partially agreed and 22% (rather) not agreed.

[What I liked most about CC was that...] it was not about working with wooden models and boring blackboard calculations.

This numbers show that students had mixed feelings about the use of CC. One explanation may be that 28% (rather) agreed and 33% partially agreed that they were not quite sure what to do with the program sometimes. One student concluded:

Good for a deeper insight from upper high school onward, but can be overwhelming/not good for everyone

Several students mentioned that they would prefer to implement the CCL in the classroom with the help of teachers:

funny, exciting - much better with teacher explanation

STRATEGIES OF STUDENTS WORKING WITH THE CCL

While the first part focused on the usability of the CCL, the next chapter investigates how students use the CCL to solve chemical problems. Therefore, the problem-solving strategies of students working with the CCL was analyzed. Note that only student data from cycles 2 and 3 were analyzed as outlined in Methods.

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Table 1. Students' Problem-Solving Strategies for Task 1: "What is the Distance between Two Chlorine Atoms in a Chlorine Molecule (Cl2)?"

Focus group	*Problem-solving strategy sequence*[a]					*Hint energy minimum*[b]	*Task solved*[c]
2A	t&e	zero	geom.	min.		yes	
2B	zero	t&e	zero			yes	
2C	t&e	zero	min.	zero	min.	yes	yes
2D	t&e	zero	t&e	zero	min.	yes	yes
2E	init.	t&e	min.			yes	yes
2F	init.	t&e	geom.	t&e	zero	yes	no
3A	init.	max.	zero	min.		yes	yes
3B	init.	t&e	zero	min.			yes
3C	t&e	zero	max.	min.		yes	yes
3D	init.	zero	geom.	min.		yes	yes
3E	init.	zero	min.				
3F	init.	zero	min.			yes	yes

[a]Strategies as described in the text and in the codebook (SI): t&e = trial-and-error; zero = searching for point zero; init. = assuming the initial distance; max. = searching for a maximum; min. = searching for a minimum; geom. = trying prominent geometries. [b]Students received a hint to look for the energy minimum as the most stable state. [c]Students found the correct distance. Fields in orange indicate that students found the answer without explicitly referring to an energy minimum.

Problem-Solving Strategies for Two-Atomic Systems

The first two tasks (Box 1) focused on the chlorine molecule. Table 1 shows that the students consistently employed similar problem-solving strategies.

Assuming the Initial Distance. Seven of the 12 groups initially proposed the arbitrarily chosen chlorine-chlorine distance of 509 pm in the molecule representation as the correct solution. Only after receiving feedback from the adaptive system or from the TA did the students begin to use the CC calculations.

Trial-and-Error. After having excluded the initial distance, nine groups relied on a trial-and-error method to find the correct answer.

1: Make it very far apart.
[Calculation 814 pm, 569 pm, 435 pm, 294 pm, 152 pm, 36 pm]
1: Why was that just at seven? Pretty close and then pretty high number.
[Calculation 6 pm]
2: What are you doing?
1:20 000 kJ/mol. The closer it comes together, the greater the energy.
2: The distance gets bigger here, and the energy also gets bigger, yes. But also [when the atoms come] closer. (2D, see Figure 7)

The example of group 2D illustrates well how obtaining data through a trial-and-error approach helps students tackle a scientific problem. The students attempted to predict how the curve would behave. This process begins at the level of purely describing the depicted graph. Several students did not activate cognitive resources related to chemical structure during this phase but instead focused on superficial and mathematical features. Others, like group 2D, began to connect the energy values to structural features such as the distance.

Trying Prominent Geometries. Other student groups focused on the structural side of the project first. They often investigated the energy of prominent looking structures:

2: Try that the two [atoms] are on the edge of each other.
[Calculation 351 pm]

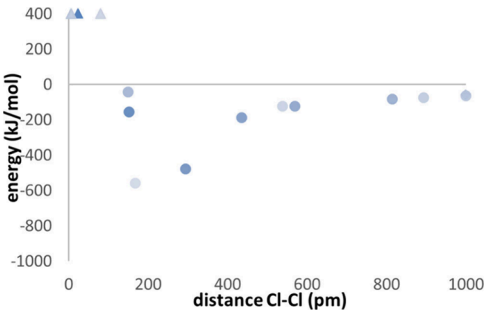


Figure 7. Data points of group 2D in their trial-and-error phase. The darker the color of the marker, the later the corresponding data point was calculated by the students. Triangles indicate that the energy value is much higher than the scale allows.

2: Oh ok (disappointed) (2A)

The students using this strategy mainly seemed to be looking for unusual geometries. Mostly, they did not argue from a chemical point of view why these geometries might be of special interest.

Searching for a Maximum. Most groups focused on energy values rather than on the structural features of the molecule. For example, two groups searched for a maximum of the graph.

2: Oh ah okay! I got it. There are different distances. We should see which has the highest energy.
1: I seeee!
[Calculation 434 pm] (3A)

These groups followed their strategy until they received feedback that searching for a maximum did not move them in the right direction. However, students started trying to make sense of calculated energy values. This allowed them to make an initial connection between the energy and chemical structure.

Searching for Point Zero. All but one group looked for the zero point of energy at some point in their problem-solving process. Figure 8 shows an example of how group 2F went all the way to a distance of 16 000 pm to find a structure with an energy

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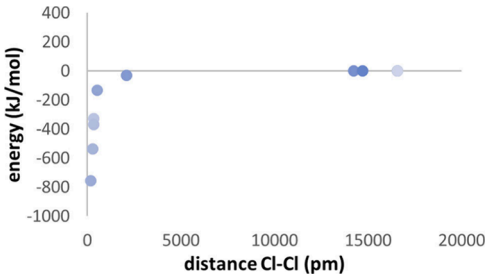


Figure 8. Data points of group 2F looking for point zero at very long distances.

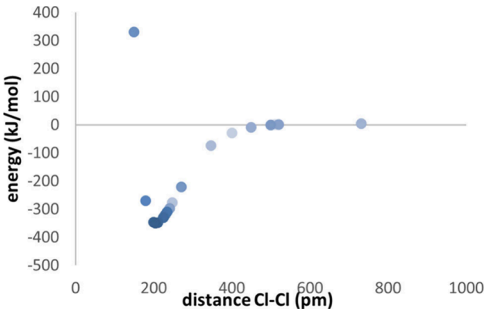


Figure 9. Data points of group 3B showing a systematic approach to find the energetic minimum. The darker the color of the marker, the later the corresponding data point was calculated by the students.

value of zero, although the resulting representation no longer resembles a molecule. Other groups looked for "zero energy" at the intersection of the graph and the *x*-axis at a distance of 50 pm.

Many students seemed to rationalize their approach by equating an energy value of zero with "no energy" and stability:

1: I want to get this to zero.
[Calculation 1075 pm]
1: I do not think I can get this to zero.
2: Never.
[Calculation 1197 pm, 1382 pm]
2: You'll never get it done.
[Calculation 1569 pm]
1: The distance they normally have will be the distance where they have no energy, right? (2B)

Searching for a Minimum. None of the groups were looking for a minimum from the beginning. However, by the end of the work phase, 10 out of 12 student groups were able to use this strategy. Only group 3B derived this strategy without a specific hint:

1: I do not understand the meaning right now. Would the most stable simply not mean zero?
2: I thought so too. But maybe not. They want to release energy.
3: The least energy is the most stable.
2: But it does not want zero either.
3: Yes, minus! Negative value!
2: Okay, that means that we find the most negative value. That means somewhere here, it should be even smaller. So, try 270 [pm]? (3B)

This example well illustrates how students begin to question their problem-solving strategy based on CC data. They rediscuss the concept of stability and realize that negative energy values could represent an even more stable state than "zero energy". Having made this connection, the group searches for the minimum in a very strategic way, as shown in Figure 9.

All other groups needed a clear hint that solving the task required finding the most stable state, which corresponds to the lowest energy. For many, this insight was a game-changer, and they quickly shifted to searching for the minimum.

[Hint minimal energy]
1: That means that we want the energy to be as small as possible. [...]
3: That means we'll just have the energies calculated each time, roughly around that distance, and where we then have the largest negative energy, that's it... I guess. (3D)

Some groups, however, seemed to follow the recipe of the hint without further reflection of its background. Hence, they seemed to solve a mathematical problem rather than a chemical problem.

1: So at 200, is there such a low point?
2: There is a kind of asymptote. (2A)

Some of these groups reflected their solution afterward. In the following example, while Student 3 initially struggled to understand the approach, they quickly made new connections between energy and stability during the discussion.

3: But nobody would think of that [solution].
2: Yes, they do.
3: Oh, because we want to have little energy. Zero would be a lot. (3E)

Task 2 asked for the energy required to split a chlorine molecule. The answer is easy to read from the already calculated curve. All groups except group 3D made the transfer. Some of the groups needed guidance on the correct sign of the energy value.

Transfer to Three-Atomic Systems

After working on the chlorine molecule, students were asked to investigate a three-atom system (see Box 1). This increases the level of difficulty, requiring students to adapt their strategies to a new problem. Table 2 gives an overview of students' strategies in this novel context.

Applied Problem-Solving Strategies. Four groups started with a trial-and-error approach or tested conspicuous geometries. In contrast to the first task, none of the groups focused on finding point zero. Unsurprisingly, many student groups quickly started looking for an energy minimum, reflecting the strategies that they had developed during the first task. The true transfer of knowledge emerged when students interpreted this first minimum as representing the reactants and began searching for a second minimum energy corresponding to the reaction products.

2: Do you think there's a second dip?
1: Yes.
2: Let's try it directly. (3B)

Others described their approach directly after reading the task.

1: Now we find out where that [points to reactants' structure] has its lowest point, and then we find out where that [points to products' structure] has its lowest point or what? (2B)

To investigate the activation energy, the students had to find a maximum corresponding to the transition state. Eight of the 12 groups also succeeded in finding that point.

1: So, we already have the energy of the reactants.
2: So, we just have to find the highest ...
1: ... the highest point of the curve. (2D)

Modeling. One new strategy emerged that was not observed in the earlier task. Some students modeled the reaction at the

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Table 2. Overview of Students' Problem-Solving Strategies for Calculating the Released Energy and Activation Energy in a Reaction of a Chlorine Molecule and Hydrogen Radical (See Box 1)

Focus group	*Problem-solving strategy sequence*[a]					*Key hint*[b]	*Released energy*	*Activation energy*
2A	t&e	model.	max.			yes		
2B	min. 1	min. 2	min. 1	min. 2	max.	yes		
2C	min. 1	min. 2						
2D	model.	min. 2	max.			yes		
2E	model.	min. 2	max.	model.				
2F	t&e	model.	t&e	max.	model.	yes		
3A	min. 2	max.						
3B	min. 1	t&e	min. 2			yes		
3C	max.	min. 2				yes		
3D	t&e	geom.	model.	geom.	max.			
3E	geom.	t&e					guess	
3F	min. 1	model.				yes		

[a]Strategies as described in the text and in the codebook (SI): t&e = trial-and-error; max. = searching for a maximum; min. = searching for a minimum; geom. = trying prominent geometries; model. = modeling the reaction. [b]Students received a hint to find the energy of reactants and products.

submicroscopic level before proceeding to calculate the corresponding energy values.

2: Yes, should the H and the Cl not be more together?

1: Ahh, that's exactly what happens, that the [...] Cl splits off from Cl and goes to the H.

2: We can calculate it. (2A)

Solving the Tasks. Students were tasked with calculating the released energy and activation energy of the reaction step. Two groups were unable to arrive at a solution. Both of these groups also struggled with the first task and were, at times, not working with full concentration. Group 3E managed to find the correct solution by strategically using the feedback system, although without activating relevant chemical cognitive resources.

All other groups successfully computed both the released energy and the activation energy from the CC results. Some groups were able to use CC to answer the questions in a highly strategic way, even without external support.

1: That means we are now also looking for...

2: H and Cl_2, which then has an energy of... [...]

2: Um, then HCl and Cl. [...]

2: 419. then the difference thereof. (2C)

Many students used the adaptive feedback system. One particular hint proved to be of particular significance for many students. Their key breakthrough occurred when they were explicitly prompted to connect the energy values to the reactants and products.

1: This [pointing to 1st minimum] is the energy from the reactants, and this [pointing to 2nd minimum] is from the products, I would say.

2: So, we are quite good up to here. That means we form the difference between this and that. (2B)

■ DISCUSSION AND IMPLICATIONS

The central finding of this study is that high school students can use CC as a tool for scientific inquiry when they are supported appropriately. Students quickly learned how to navigate the platform and used the calculated energy values to explain chemical reactions. Implementing CC in the chemistry classroom comes with great potential to foster scientific understanding, use authentic modern scientific inquiry methods, and use digital media in a meaningful way.

CC Environments for High School Students Should Be Tailored Based on Empirical and Scientific Analysis

The described DBR process highlights that a CC environment must be carefully designed to allow meaningful learning. The design should be based on rigorous scientific analysis. In the case of QC, this specifically involves the search for an appropriate level of quantum theory. For the reaction investigated here, only a suitable level of theory allows the calculation of meaningful bond dissociation energies. Only with this accuracy is it possible to discuss the experimental finding that red light does not initiate a chain reaction but blue light does.

A second requirement is to base such innovations on empirical data. For example, our observations showed what support students need to make learning with CC meaningful. This includes encouraging students to activate relevant prior knowledge and to make new connections. In this project, this was realized via rule-based adaptive feedback. Observations and student feedback indicates that this adaptive feedback is highly valued and helps students to work with the program in a meaningful manner.[10]

The results suggest that the learning environment developed can address several of the challenges for implementing CC in the classroom outlined by Tuvi-Arad:[36] The Comp-Chem-Lab (CCL) makes the infrastructure of CC accessible, eliminates the need for technical training, and can be used by teachers with little knowledge of CC. These advantages come at the cost that the CCL limits the use of CC to a very specific problem and neglects the theoretical background. Therefore, the suitability of CCL depends heavily on the specific learning goals set by the teacher. A remaining challenge is teachers' self-efficacy and beliefs: In the DBR process, many teachers were much more critical of the use of CC in schools than the students who actually use it.

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For future research, it is desirable to develop design principles for constructing CC learning environments in high schools. This involves questions on different forms of representations of entities,[56,57] suitable analysis methods, more adaptive support, e.g. using generative AI,[54,55] and ways to reduce the complexity of the results in an appropriate manner. Furthermore, future research should focus on how the use of CC affects learning processes and scientific inquiry skills in real chemistry classrooms.

Does Using CC Experiments Improve Students' Understanding of Energy?

Many students in our sample activated similar energy-related resources as observed in previous studies.[2,20,58] Notably, the idea that a state with "no energy" is stable was particularly dominant among students. This could stem from the fact that the standard enthalpy of formation for molecular chlorine, as the most stable form of its element, is commonly set to zero. Students may have drawn on this idea that is taught in the curriculum. Additionally, they avoided discussing negative energy values. Consistent with findings from other studies,[59] students appeared to lack a clear conceptual understanding of negative energy. The underlying issue seems to be that students are unaware that discussions about energy inherently involve energy differences. Working with CC could help raise this awareness, as determining a reasonable reference energy is a fundamental aspect of CC (see eq 1). To reduce confusion, it would be beneficial to clearly address which energy difference is used.

It is particularly striking that none of the students directly activated the idea of (potential) energy minimization. Most students grasped this concept only after receiving a direct hint. Interestingly, the principle itself does not appear to be particularly challenging for them. Many students were able to not only apply it successfully in the initial task after receiving the hint but also transfer it to subsequent tasks with little difficulty. This may suggest that the problem lies in the lack of emphasis on this fundamental concept in the current curriculum. One consequence of this lack is that students often rely on the octet rule or other heuristics.[26,30] Alternative teaching approaches, such as a force-and-energy perspective on chemical bonding, were already found to enhance students' understanding of energy.[58,60−62]

In agreement with our results, Hrubeš et al.[6] found that high school students are able to discuss bond lengths based on QC data. Their approach was to teach QC principles to high-achieving students and then to use Gaussian software directly. While the original software may provide more authentic insights into scientific research tools, a prestructured environment, such as the one used in this study, may allow students to experiment more flexibly. In addition, the purposefully designed environment here allows high school students to investigate more complex reactions than the authentic environment in Hrubeš et al.'s study. While Hrubeš et al. showed how well-trained teachers can teach the basics of QC to high school students, the CCL allows QC to be used without the availability of QC experts. However, this comes at the cost of providing less insight into the QC calculations. It would be of great value to compare empirically how these different approaches affect student learning.

The results suggest that working with CC has the potential to trigger conceptual change in students. Specifically, it appears to strengthen the critical connection between the chemical structure and energy, a link that is often weak in student understanding. The method of this exploratory study does not allow for definitive conclusions about the conceptual change. More research is needed to investigate the impacts of CC on students' conceptual knowledge using an interventionist approach in an authentic school context.

Does the Use of CC Give Students Insight into the Role of Simulation in Scientific Inquiry?

One of the primary goals in developing the CCL is to help students recognize that model-based simulations, particularly those based on QC, play a significant role in generating new insights in chemistry. The present study did not explicitly investigate how far students were able to differentiate CC as a model-based scientific inquiry method from interactive animations. However, some aspects could suggest that students have gained initial awareness of this concept.

Initially, many students did not seem to realize that simulations could be used to address scientific questions. For example, their assumption that the initial distances in the molecular models were correct suggests that they may have perceived simulations as mere visualizations. In the CCL, however, students quickly began to use simulations for inquiry. Many adopted algorithmic problem-solving strategies, using CC data to interpret phenomena and test hypotheses, which may indicate the emergence of computational thinking.[63]

Despite careful screening of the methods, the potential energy curves in the CCL exhibit some irregularities. These disruptions might seem problematic, because they draw attention to secondary aspects. From another point of view, they could also offer valuable learning opportunities. Understanding deviations is fundamental to CC, which—like all scientific inquiry—is based on models with inherent limitations.[12] Idealized graphs commonly found in animations, textbooks, or educational materials can foster unrealistic views of science. In contrast, working with authentic, imperfect data could help students develop a more accurate understanding of scientific inquiry.

This study does not aim to make definitive claims about the development of these competencies. However, enabling students to engage with real scientific data, including its limitations, is one of CC's greatest potentials in high school education. Future research should explore in detail how CC influences students' epistemological beliefs and computational thinking competencies.

■ LIMITATIONS

The presented study is of an exploratory nature. It is not intended to be proof of the suitability of CC as a learning environment in high school. Instead, they qualitatively investigate the feasibility in a specific context.

The study was conducted in an out-of-school laboratory, whereas DBR research is usually conducted in chemistry classrooms. The environment is designed to look as much like a chemistry classroom as possible. However, intervention still has to be implemented in the more complex reality of a chemistry classroom.

The CCL including the adaptive feedback system was developed for German students in 11th grade. The capability and preknowledge may differ in other educational systems. The capacity and computing power of the CCL is still limited, which could cause problems in case of many users.

QC is used as a black box in the CCL. For future research, a stronger focus on the principles of QC should be implemented

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to provide deeper insights into the origins of the different energies.

CONCLUSION

A design-based research approach was employed to develop a platform that enabled high school students to conduct computational chemistry (CC) experiments. An appropriate choice of CC methods, an adequate reduction of complexity, and the empirical investigation of students' needs have proven to be especially important to consider when developing such implementations. Prominently, it is crucial to provide students with suitable analytical tools and adaptive feedback.

Students used an archetypal pattern of problem-solving strategies to investigate the energetic aspects of the reaction between molecular chlorine and hydrogen. They used CC data to make claims about chemical reactions, applied algorithmic strategies to test their hypotheses, and developed new strategies based on CC results. In short, they used the CC for scientific inquiry.

The findings along with other recent studies[6,7] can serve as proof of concept that high school students can effectively engage with CC when it is presented appropriately. To realize the full potential of CC in chemistry education and to advance the field, a broad range of basic research is needed. This should include the tailored development of CC learning environments, the study of CC in a variety of authentic learning environments, and empirical studies of how the use of CC impacts students' conceptual knowledge, epistemic beliefs, and science inquiry skills.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.4c01136.

Survey instruments, code system of the content analysis, evaluation results, details on the screening of levels of theory, original quotations in German, further details on the DBR process (PDF)

Student worksheet (PDF, DOCX)

AUTHOR INFORMATION

Corresponding Author

Benjamin Pölloth − *Freie Universität Berlin, Berlin 14195, Germany;* orcid.org/0000-0001-7777-9903; Email: benjamin.poelloth@fu-berlin.de

Complete contact information is available at: https://pubs.acs.org/10.1021/acs.jchemed.4c01136

Notes

The author declares no competing financial interest.

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