

# Interactive simulations to support quantum mechanics instruction for chemistry students

Antje Kohnle\* and Cory Benfield<sup>a</sup>

School of Physics, University of St Andrews, St Andrews, KY16 9SS, United Kingdom

5 <sup>a</sup>now at Hewlett Packard Enterprise, Filton Road, Stoke Gifford, BS34 8QZ, United Kingdom

Georg Hähner

School of Chemistry, University of St Andrews, St Andrews, KY16 9ST, United Kingdom

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Mark Paetkau

Department of Physical Sciences, Thompson Rivers University, Kamloops, Canada V2C, OCS

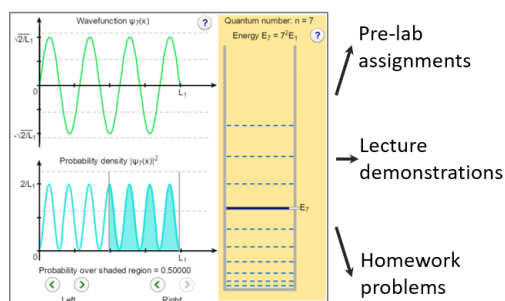
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## ABSTRACT

The QuVis Quantum Mechanics Visualization Project provides freely-available research-based interactive simulations with accompanying activities for the teaching and learning of quantum mechanics across a wide range of topics and levels. This article gives an overview of some of the simulations and describes their use in an introductory physical chemistry university course, where simulations were implemented as a pre-lab assignment, as lecture demonstrations, and as homework problems.

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## GRAPHICAL ABSTRACT



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**KEYWORDS**

First-Year Undergraduate/General, Second-Year Undergraduate, Physical Chemistry, Computer-Based Learning, Quantum Chemistry

**OVERVIEW OF THE QUVIS SIMULATIONS**

30 Quantum mechanics is fundamental to understanding atomic and molecular structure and spectra and chemical bonding, but its mathematical complexity and often counterintuitive consequences such as the wave-like behavior of particles can present major barriers for introductory physical chemistry students. Interactive simulations have been shown to be powerful tools for chemistry instruction, through their use of  
35 macroscopic and microscopic visualizations, multiple representations and simplified and idealized situations to reduce cognitive load.<sup>1,2</sup> The interactive elements allow students to make sense of the representations shown and explore the relationships between them.

The QuVis Quantum Mechanics Visualization project<sup>3</sup> aims to support the learning  
40 and teaching of quantum mechanics through the research-based development of interactive simulations with accompanying activities.<sup>4,5</sup> Over 100 simulations are now freely available on the QuVis website, covering a wide range of topics from the introductory to the advanced undergraduate levels. Simulations include text explanations that aim to make them self-contained instructional resources. The  
45 simulations on the website are divided into two collections: older Flash simulations that run on desktop computers, and HTML5 simulations with inherent touchscreen support that are also suitable for tablets and mobile devices (one of which is shown in Figure 1). Many of the HTML5 simulations include a second “Challenges” tab with challenges aligned with the learning goals. The Challenges tab includes a score counter and gives  
50 students feedback on submitted answers. The older simulations include a second “Step-by-step exploration” tab with explanations and animated highlighting. Simulations can

be used online or downloaded from the QuVis website for offline use. Problem sets accompanying the simulations with password-protected solutions are available on the website. Instructors can edit activities as needed to suit their local context. Instructors may obtain the solutions by sending an email request.<sup>6</sup>

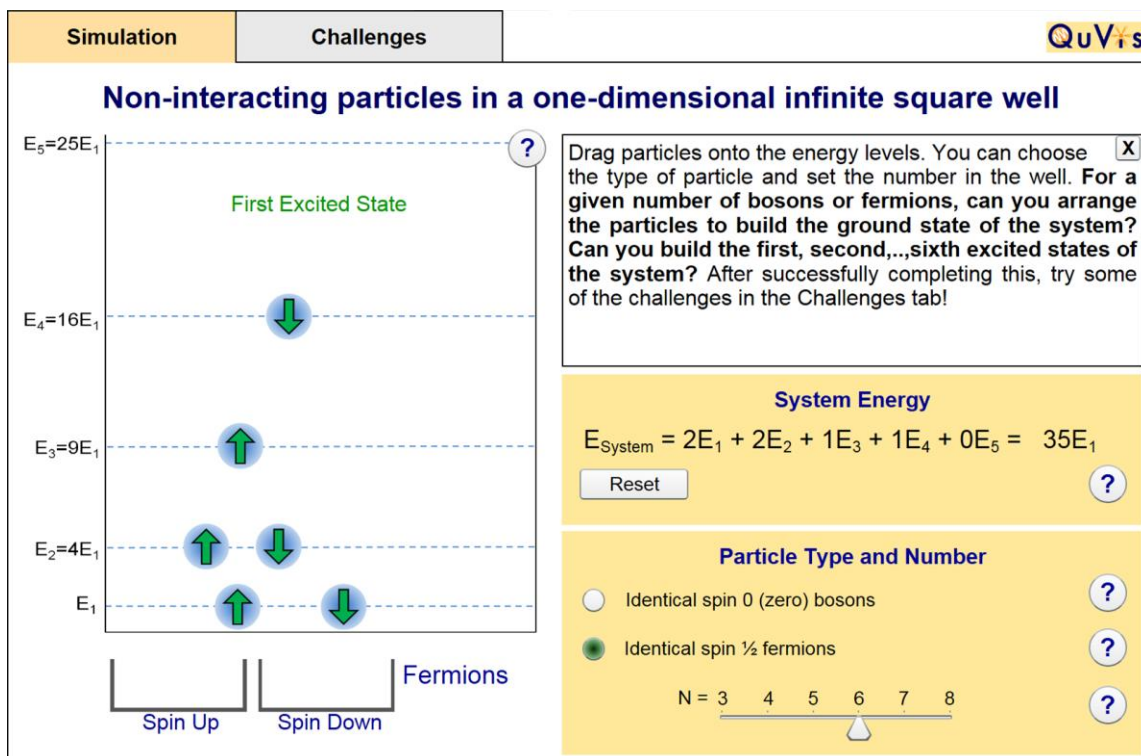


Figure 1. A screenshot of the "Simulation" view of the *Non-interacting particles in a one-dimensional infinite square well* simulation.<sup>15</sup>

60 Simulations are based on our research and the literature on student difficulties with quantum mechanics.<sup>7-10</sup> They make use of implicit scaffolding<sup>11</sup> by guiding students towards the learning goals through the visualizations and controls available and their ranges and layout. They are based on principles of perception-based interaction design<sup>12</sup>, such as the use of intuitive controls, using color to highlight objects and link  
65 different representations and grouping controls with similar functions. After development, simulations are tested with individual student volunteers and iteratively refined based on student and instructor feedback. Evaluation with in-class trials

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includes the use of student surveys, pre- and post-tests and analysis of students' success in completing the simulation activities.<sup>4,5,13</sup> The Supporting Information

70 includes further details on simulation design and refinement as well as website features and navigation.

### **SIMULATION USE IN AN INTRODUCTORY PHYSICAL CHEMISTRY COURSE**

QuVis simulations have been used to support student learning in an introductory physical chemistry course at the University of St Andrews since 2012. The course is typically taken by 90 students in their second year of study and includes class time, homework problems and two lab sessions per week. The quantum mechanics part of this course provides an introduction to the quantum mechanics of atoms. Topics covered include de Broglie matter waves, the time-independent Schrödinger equation and the Born interpretation, the Heisenberg Uncertainty Principle, the particle in a box (the infinitely-deep potential well), the finite-depth potential well, identical particles and the Pauli Principle, quantum numbers, orbitals and energy levels for the hydrogen atom, spin angular momentum, the building-up principle of many-electron atoms, spin-orbit coupling and selection rules for transitions between energy levels. In what follows, we describe how simulations were implemented into this course to support instruction.

80 Simulations are given by their full title, with the short title used to list simulations on the website in parentheses and the URLs in the references. The Supporting Information includes a syllabus of topics with all simulations used.

#### **Simulations as pre-lab assignments**

Two simulations, *Wavefunctions and energy levels of a particle in a one-dimensional box*<sup>14</sup> (1D Particle in a Box) and *Non-interacting particles in a one-dimensional infinite square well*<sup>15</sup> (Particles in an Infinite Well) were used as a pre-lab assignment for a lab experiment on the absorption spectra of conjugated systems. A screenshot of the latter simulation is shown in Figure 1. This simulation allows students to place identical spin

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1/2 fermions or spinless bosons into the same infinite well to build the ground state,  
95 first excited state, etc. of the system. Thus, students observe that the energy for a  
system of multiple quantum particles is the sum of the individual energies. In addition,  
if students try to place two fermions with the same spin orientation on the same energy  
level, one fermion drops down into the container below the well. This observation allows  
students to discover the Pauli principle, that a maximum of two fermions (one with  
100 spin-up, one with spin-down) can occupy each energy level.

The pre-lab assignment was set up as an online quiz. Students use the simulation  
shown in Figure 1 to determine the electron configurations and total energies for a  
molecule with 4, 6 and 8  $\pi$ -electrons using the infinite square well model. They then  
determine the UV photon absorption energy needed to promote the molecule from the  
105 ground state to the first excited state, by promoting an electron from the highest  
occupied energy level to the lowest unoccupied level.

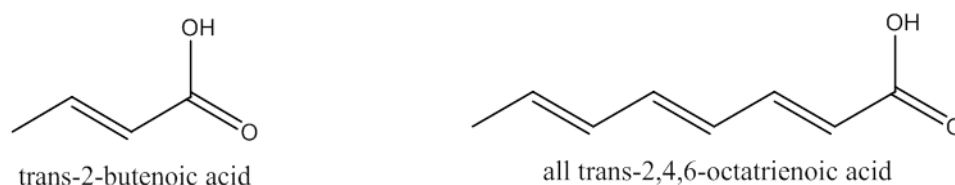


Figure 2. Two conjugated molecules of different length, experimentally studied in the lab and modelled as described in the  
text using the particle in a box model.

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In the lab experiment, students measure the UV absorption of a series of conjugated  
molecules of different length, such as the ones shown in Figure 2. The particle in a box  
model is used to estimate the absorption wavelength based on the assumption that the  
 $\pi$ -electrons are free to move along the length of the molecule. The pre-lab assignment  
115 ensures that students understand a simple theoretical model that can be used to  
describe the experiment. They learn for example that the absorption wavelength will  
depend on the length of the molecule (i.e. the length of the box) and are able to judge if

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the trend observed in the experiment is correct. The final data evaluation is done in the written report. Students are then also asked to consider the accuracy of the

120 theoretically determined values and to discuss potential sources for the observed deviations between experiment and model (limitations of the model; deviation of molecules from the particle in a box model etc.).

#### Simulations as in-lecture demonstrations and as homework problems

125 Simulations are also used to illustrate concepts in class and to help students visualize concepts in homework problems. The physical chemistry course is taught through traditional lectures. Simulations are employed by the instructor during the lecture to support concepts in quantum mechanics that are considered to be difficult by many students. As lecture time is limited, students are encouraged to explore the simulations in more detail outside of class time. In what follows, we give some

130 examples of how simulations are used in the lectures; the Supporting Information includes a full list of simulations used in the lectures and as homework problems. They are presented in the order in which they appear in the course.

Many chemistry students are not familiar with eigenfunctions and eigenvalues, concepts that underpin the Schrödinger equation. The *Graphical representation of*

135 *eigenvectors*<sup>16</sup> (Eigenvectors and Eigenvalues) simulation is used by the instructor during the lecture to help students make connections between graphical and mathematical representations of eigenvectors and eigenvalues. The simulation depicts the two components of a unit vector in the xy-plane, and the same vector under several different transformations. The orientation of the initial vector can be changed using a

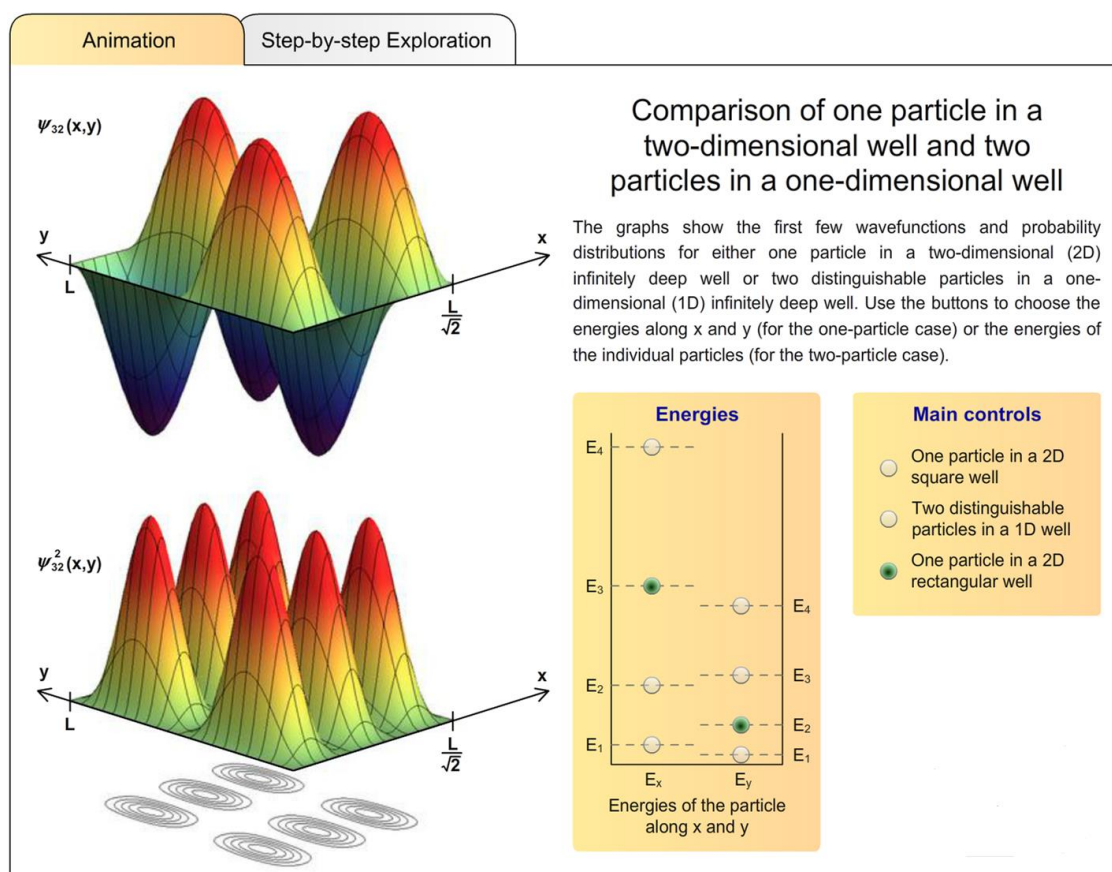
140 slider. The simulation shows whether or not the vector is an eigenvector, and if so displays the associated eigenvalue.

Another example is the interpretation of the modulus squared of the wave function as a probability density (also called a probability distribution). In order to illustrate

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probability density using a classical system well known to students, the *Probabilistic analysis of a mass-spring system*<sup>17</sup> (Classical Oscillator) simulation is employed. The simulation allows users to take snapshots at random times of the position of a mass on a spring, and displays the probability density of the resulting position distribution. The simulation thus demonstrates how a probability density can be obtained for a classical system.

150 The course discusses the particle in a box (the infinitely-deep potential well) in one and more dimensions. This part of the course uses the *Comparison of one particle in a two-dimensional well and two particles in a one-dimensional well*<sup>18</sup> (1D and 2D Infinite Well) simulation shown in Figure 3. It allows users to compare the probability distribution for a single quantum particle in a two-dimensional square well or  
155 rectangular well, and the probability distribution for two particles in a one-dimensional infinite well. The simulation is used in the course to introduce degeneracy by showing that different combinations of quantum numbers can give the same total energy though the wavefunctions are different. It is also used to introduce the symmetry or antisymmetry requirements of quantum-mechanical wavefunctions describing several  
160 identical particles (fermions and bosons), by demonstrating that otherwise the probability density at a certain position would not be identical if the labels of two particles with different energies are swapped.



165 Figure 3. A screenshot of the *Comparison of one particle in a two-dimensional well and two particles in a one-dimensional well*<sup>18</sup> simulation. For the view shown, the user can choose the energies  $E_x$  and  $E_y$  of the particle along  $x$  and  $y$ . The total energy of the particle is given by the sum  $E_x + E_y$ .

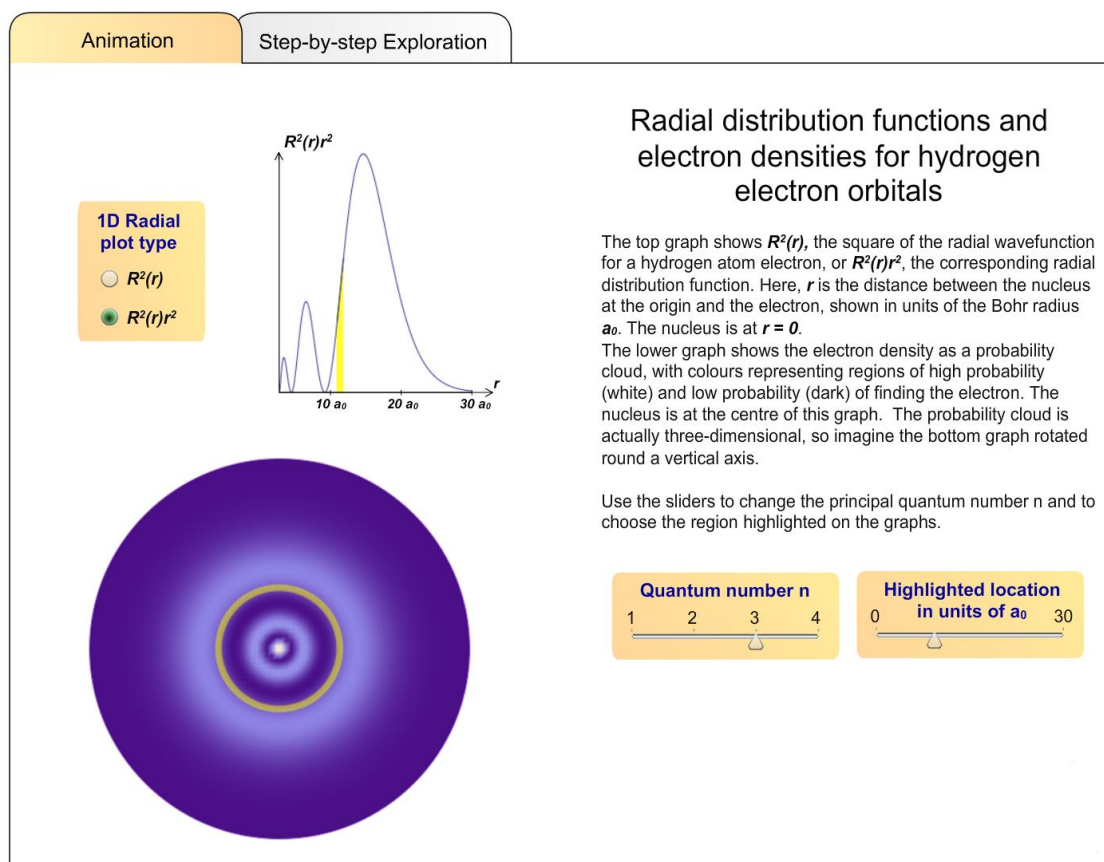
The course introduces the orbitals and energy levels for the hydrogen atom. The *Radial distribution functions and electron densities for hydrogen electron orbitals*<sup>19</sup>

170 (Radial Distribution Functions) simulation shown in Figure 4 is used in this part of the course to help students translate between the three-dimensional electron density representation and the radial distribution function for the hydrogen atom. A highlighted region can be moved in both graphs to better compare them. The visualization during the lecture helps students to differentiate between the most likely point in space to find

175 the electron (this would be the origin for the state shown in Figure 4) and the most



likely radial distance to find the electron (the maximum of the radial distribution function).



180 Figure 4. A screenshot of the *Radial distribution functions and electron densities for hydrogen electron orbitals*<sup>19</sup> simulation.

The *Experimental proof of spin angular momentum: The Stern-Gerlach experiment*<sup>20</sup> (Experimental Proof of Spin) simulation is used to introduce spin angular momentum. With the help of this simulation, students are led from the classical expectation to the  
185 quantum result. The simulation allows users to compare the experimental outcomes of a Stern-Gerlach experiment for classical rotating particles, quantum particles with orbital angular momentum, and quantum particles with spin 1/2 angular momentum. The *Semi-classical vector model of orbital angular momentum*<sup>21</sup> (Vector Model Angular Momentum) simulation is used to help students visualize the quantized nature of

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190 orbital angular momentum. It depicts orbital angular momentum vectors and cones of possible angular momentum directions. The quantum numbers for the magnitude and the z-component of angular momentum can be changed.

## CONCLUSIONS

The QuVis simulations can support quantum mechanics instruction for physical chemistry students. This article has described their use as in-class demonstrations, 195 homework problems and pre-lab activities, and given examples of simulations used in an introductory physical chemistry course. The simulations and accompanying activities are freely available on the QuVis website. Further development of simulations (including the recoding of the Flash simulations described in this article in HTML5) and 200 evaluation and refinement through instructor and student feedback are ongoing.

## ASSOCIATED CONTENT

### Supporting Information

Syllabus of the Physical Chemistry course with topics and all simulations used, further information on the research-based simulation development process, general 205 guidelines for simulation use, and website features and navigation (PDF)

## AUTHOR INFORMATION

### Corresponding Author

\*E-mail: ak81@st-andrews.ac.uk

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an HTML5 version, available at [http://www.st-](http://www.st-andrews.ac.uk/physics/quvis/simulations_html5/sims/infwell1d/infwell1d.html)

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