QIS Key Concepts for K-12 Chemistry

Framework for K-12 Quantum Education

The world is in the midst of a second quantum revolution due to our ability to exquisitely control quantum systems and harness them for applications in quantum computing, communications, and sensing. Quantum information science (QIS) is an area of STEM that makes use of the laws of quantum physics for the storage, transmission, manipulation, processing, or measurement of information.

After the passage of the US National Quantum Initiative Act in December 2018 [1], the National Science Foundation and the White House Office of Science and Technology Policy (WHOSTP) assembled an interagency working group and subsequently facilitated a workshop titled "Key Concepts for Future Quantum Information Science Learners" that focused on identifying core concepts essential for helping pre-college students engage with QIS. The output of this workshop was intended as a starting point for future curricular and educator activities [2-4] aimed at K-12 and beyond. Helping pre-college students learn the QIS Key Concepts could effectively introduce them to the Second Quantum Revolution and inspire them to become future contributors and leaders in the growing field of QIS spanning quantum computing, communication, and sensing. The framework for K-12 quantum education outlined here is an expansion of the original QIS Key Concepts, providing a detailed route towards including QIS topics in K-12 physics, chemistry, computer science and mathematics classes. The framework will be released in sections as it is completed for each subject.

As QIS is an emerging area of science connecting multiple disciplines, content and curricula developed to teach QIS should follow the best practices. The K-12 quantum education framework is intended to provide some scaffolding for creating future curricula and approaches to integrating QIS into physics, computer science, mathematics, and chemistry (mathematics and chemistry are not yet complete). The framework is expected to evolve over time, with input from educators and educational researchers.

Why quantum education at the K-12 level?

Starting quantum education in K-12 provides a larger, more diverse pool of students the opportunity to learn about this exciting field so that they can become the future leaders in this rapidly growing field. This is especially important because over the past century during which the first quantum revolution unfolded, the quantum-related fields have lacked gender, racial, and ethnic diversity. We must tap into the talents of students from diverse demographic groups in order to maintain our leadership in science and technology. Early introduction to quantum science can include information on applications and societal relevance, which will hopefully spark excitement and lead more students into later coursework and careers in STEM. Also, starting early with a conceptual, intuitive approach that doesn't rely on advanced mathematics will likely increase quantum awareness with more students, even those who do not pursue a career in QIS. In the long term, this will potentially improve public perception of QIS, moving it out of the weird, spooky, incomprehensible, unfamiliar realm.

What are some considerations to take into account when introducing QIS into the K-12 classroom?

As an emerging field that has traditionally been the realm of advanced undergraduate and graduate study with an aura of complexity, educators designing and delivering curriculum should keep the following in mind when integrating QIS into their classrooms.

1. Because existing materials in QIS are designed for more advanced students, the materials need to be adjusted to be age-appropriate for and build on prior knowledge of target students. As new educational research and data on implementation come in, the materials will change and improve over time.
2. Because the area may be intimidating, and there is no expectation in college that students have already learned this, motivational goals such as higher self-efficacy and a sense of belonging and identity [5-11] should be on equal footing with technical goals. Therefore, classrooms should focus on the following considerations:
    - Maintain a supportive atmosphere that encourages questions and exploration
    - Offer collaborative, exploratory activities
    - Offer a low-stakes educational setting (e.g. little time pressure without aggressive testing)
    - When relevant to the STEM subject, employ a learning cycle approach to develop models of quantum systems and phenomena, plan and carry out investigations to test their models, analyze and interpret data, obtain, evaluate, and communicate their findings

QIS K-12 Key Concepts Chemistry Focus Group

Quantum information science leverages quantum mechanics to develop new capabilities in computing, sensing, and communications. In many chemistry classes, there may be natural points of integration around topics such as atomic and molecular structure, orbitals, spectroscopy, and electron configuration. The purpose of the QIS K-12 Key Concepts Chemistry Focus Group was to create an initial set of expectations and learning goals, which will be useful to curriculum developers and teachers seeking to develop chemistry lessons and activities for teaching QIS K12 Key Concepts.

The focus group brought together a range of experts, including educators familiar with both teaching and research of physics concepts at high school and/or university levels. The members were:

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- *Emily Edwards, University of Illinois Urbana-Champaign, Urbana, IL
- Jim Hall, Cedar Ridge High School, Round Rock, TX
- Scott Hawkins, St. Ignatius High School, Cleveland, Ohio
- Kevin Lavigne, Hanover High School, Hanover, NH
- Olayinka Mohorn, Dominican University, Chicago, IL
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- John Phipps, Hanover High School, Hanover, NH
- *Chandralekha Singh, University of Pittsburgh, Pittsburgh, PA
- Jennifer Smith, Illinois Virtual School, Peoria IL
- Jeanette Stewart, Marist School, Atlanta, Georgia
- Heather Weck, Harriton High School, Rosemont, PA
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*Designates working group leads, conveners, and/or framework editors.

The output from this group was a series of expectations and outcomes for each QIS Key Concept. This initial framework is intended to evolve over time as quantum education for K-12 develops.

1. QUANTUM INFORMATION SCIENCE

Quantum information science (QIS) exploits quantum principles to transform how information is acquired, encoded, manipulated, and applied. Quantum information science encompasses quantum computing, quantum communication, and quantum sensing, and spurs other advances in science and technology.

a. Quantum information science employs quantum mechanics, a well-tested theory that uses the mathematics of probability, vectors, algebra, trigonometry, complex numbers, and linear transformations to describe the physical world.
b. Quantum information science combines information theory and computer science, following the laws of quantum mechanics, to process information in fundamentally new ways.
c. Quantum information science has already produced and enhanced high-impact technologies such as the Global Positioning System (GPS), which depends on the extreme precision of atomic clocks based on the quantum states of atoms.

The definition of QIS could be discussed as a precursor to any of the other concepts, or in discussions of career opportunities in the field.

2. QUANTUM STATE

Key Concept:
A quantum state is a mathematical representation of a physical system, such as an atom, and provides the basis for processing quantum information**.**

- Quantum states are represented by directions or vectors in an abstract space.
- The direction of the quantum state vector determines the probabilities of all of the possible outcomes of a set of measurements. Quantum manipulations in the physical world follow vector operations, incorporating complex numbers and negative values. This captures a behavior of physical quantum systems that cannot be described solely by the arithmetic of probability.
- Quantum systems are fragile. For instance, measurement almost always disturbs a quantum system in a way that cannot be ignored. This fragility influences the design of computational algorithms and communication and sensing protocols.

Summary Description: A quantum state defines the properties of a quantum system, such as an electron bound to an atom. It can be represented by parameters such as quantum numbers, and contains the information needed to predict the outcomes of experiments.

Expectation: Students will describe that many properties of quantum systems are quantized, meaning that they are restricted to discrete values, and explain experimental evidence for quantization.

Learner Outcomes

1. Students will be able to identify quantum states that are distinct and distinguishable.
   a. Example: A spin-up and spin-down electron have distinct quantum states.
   b. Example: An electron in the *2p* orbital is in a distinct quantum state from an electron in the *1s* orbital, and they can be distinguished from each other by their energy.
   c. Example: The *2s* and *2p* orbitals of the hydrogen atom have the same energy, but are distinct quantum states and can be distinguished by their three-dimensional shape.
   d. Example: Electrons with different sets of quantum numbers have distinct and distinguishable quantum states.
2. Students will compare and contrast quantized energy levels to continuous energy ranges.
   a. Example: The energy of an electron bound to an atom is determined by its principal quantum number “n”, which can only take integer values.

    b. Example: Electrons bound to an atom can only be in specific quantum states and energy levels corresponding to specific orbitals, such as *1s* or *2s*. Unbound electrons, such as a free electron after ionization, can have any energy.
3. Students will be able to describe the experimental evidence for quantization.
    a. Example: Atoms only emit and absorb light (photons) at specific frequencies (evidenced by their atomic spectrum), corresponding to transitions between energy levels, as can be seen with an emission tube or flame test and a spectroscope.
    b. Example: The photoelectric effect demonstrates that electromagnetic radiation consists of indivisible units, or quanta, of energy called photons.
    c. Example: Nuclear magnetic resonance (NMR) experiments show that electrons and nuclei with different spin directions have different energies when in a magnetic field, as applied in Magnetic Resonance Imaging (MRI).
4. Students will be able to describe mechanisms by which electrons can transition between different quantum states.
    a. Example: A laser at the proper (resonant) frequency can stimulate an electron from one level to a higher (excited) level.
    b. Example: An electron in an excited state will eventually relax (decay) back to a lower available orbital (energy state).
5. Students will recognize quantum states that are a superposition (linear combination) of other quantum states.
    a. Example: A hybridized orbital is a linear combination of different orbitals, and has a shape that combines features of the individual orbitals. As a specific example, in the ground state of carbon, electrons are not in the “s” orbital or the “p” orbital, but a hybrid sp3 orbital. The shape of this orbital is a linear combination of the “s” and “p” orbitals.
    b. Example: In the ground state of benzene, the bonds are alternating single- and double-bonds which can be arranged in two distinguishable ways. This hexagonal ring structure is a linear combination of these resonance structures.

3. QUANTUM MEASUREMENT

Key Concept:
Quantum applications are designed to carefully manipulate fragile quantum systems without observation to increase the probability that the final **measurement** will provide the intended result.

- A measurement is an interaction with the quantum system that transforms a state with multiple possible outcomes into a “collapsed” state that now has only one outcome: the measured outcome. *(See section on qubits)*
- A quantum state determines the probability of the outcome of a single quantum measurement, but one outcome rarely reveals complete information about the system.
- Repeated measurements on identically prepared quantum systems are required to determine more complete information about the state.
- Because of the limitations of quantum measurement (providing only partial information and disturbing the system), quantum states cannot be copied or duplicated.

Summary Description: In general, the outcome of a quantum measurement is not predetermined. The probabilities of each outcome depends on the quantum state.

Expectation: Students will describe that the results of quantum measurements are, in general, probabilistic.

Learner Outcomes

1. Students will describe atomic orbitals as probability distributions for the electron.
    a. Example: An electron bound to an atom is delocalized (spread out) before a measurement. The “shape” of the orbital illustrates the probability distribution of where the electron may be.
    b. Example: An electron in the 1s orbital has a different three-dimensional probability distribution than an electron in the 2p orbital.
2. Students will describe tools that can be used to measure the energy and other properties of electrons.
    a. Example: Spectroscopy reveals the difference between energy levels in an atom by measuring light emitted or absorbed when an electron changes energy state.
    b. Example: Emission spectroscopy measures photons (light) emitted when an electron drops in energy level, while absorption spectroscopy measures light absorbed by a sample when electrons are excited to higher energy levels.
    c. Example: Nuclear magnetic resonance (NMR) and electron spin resonance (ESR) spectra identify radio-frequency (RF) light emitted and absorbed when atomic nuclei or electrons flip their spin in a sample.

3. Students will demonstrate that quantum states can be inferred through their probability distributions by making many measurements, despite measurements on a single atom or electron being random.
   a. Example: An individual electron bound to an atom, when measured, would be in a single location rather than “spread out”. If we measure identical atoms many times, the statistics would be defined by the orbital shape (e.g., 1s). This is similar to how a single bean dropped from a jar will land in a random location, but statistics built from many beans will follow a predictable probability distribution.
   b. Example: Measuring the emission spectra of a cloud of atoms provides details about many possible transitions. An atom with a single valence electron in the excited state would only emit light of a single frequency.
   c. Example: The frequency of the photon emitted by a single atom will be described by a probability distribution given by the relative heights of the spectral peaks. After many transitions and measurements, the full spectrum can be understood.

4. QUBITS

Key Concept:
The quantum bit, or qubit, is the fundamental unit of quantum information, and is encoded in a physical system, such as polarization states of light, energy states of an atom, or spin states of an electron.

- Unlike a classical bit, each qubit can represent information in a superposition, or vector sum that incorporates two mutually exclusive quantum states.
- At a particular moment in time, a set of n classical bits can exist in only one of 2^n possible states, but a set of n qubits can exist in a superposition of all of these states. This capability allows quantum information to be stored and processed in ways that would be difficult or impossible to do classically. *(See section on quantum computing)*
- Multiple qubits can also be entangled, where the measurement outcome of one qubit is correlated with the measurement outcomes of the others.

Summary Description: A quantum bit, or qubit, is similar to a classical bit in that it can encode two states, but can also exist as a linear combination of the two states. The quantum states of electrons bound to atoms are a natural way to build qubits that can be accurately controlled and measured.

Expectation: Students will describe how quantum information can be encoded in the quantum states of electrons bound to atoms, and how this differs from classical information.

Learner Outcomes

1. Students will describe how a classical bit (binary digit) of information (0 or 1) can be encoded in a real-world object.
    a. Example: A coin can be in one of two possible states: heads or tails. We can label heads as “0” and tails as “1” to encode one bit of information into the coin.
2. Students will describe how a quantum bit (qubit) can be encoded in the state of an atom or electron.
    a. Example: The energy state of a valence electron can be in the ground state or the first excited state. We can label the ground state “0” and the excited state “1” to encode information in them.
        i. As a specific example, an electron in the ground state of the hydrogen atom is in an s orbital. Using electromagnetic radiation, it can transition to the excited state, such as a d orbital. If we restrict the electron to these two orbitals, we can use it to encode a qubit. In practice, qubits are created out of higher molecular weight atoms, but we have chosen the hydrogen atom here for its simplicity and familiarity.

    b. Example: The spin state of an electron or atomic nuclei can be spin-up or spin-down. We can label spin-up “0” and spin-down “1” to encode information in it.
3. Students will compare and contrast the properties of qubits and classical bits.
    a. Example: A qubit can be in a superposition state (linear combination) of “0” and “1”, such as a hybridized orbital.
    b. Example: A qubit, when measured, can give a random outcome of “0” or “1” according to a probability distribution depending on its quantum state.
4. Students will describe how the state of a qubit can be controlled in the lab.
    a. Example: A qubit encoded in the energy state of a valence electron can be controlled using laser beams tuned to the frequency in their atomic spectra to excite the electron to a higher energy state.
    b. Example: In a strong magnetic field, the spin-up and spin-down states of electrons have slightly different energies and can be controlled using radio-frequency fields.
5. Students will model how qubits can be measured.
    a. Example: We can measure whether an electron was in the ground or excited state by measuring whether light (photons) was emitted by the atoms corresponding to the energy difference. If in the ground state, the electron will emit no photons. If in the excited state, the electron will emit photons when it relaxes to the ground state.
    b. Example: A qubit in a superposition (linear combination) state, when measured, will be found to be “0” or “1” randomly. If encoded in the energy state of an atom, we will have some probability of detecting no photons (“0”) and some probability of detecting photons (“1”) corresponding to the quantum state of the electron. Each measurement gives one classical bit of information.
6. Students will use the periodic table to predict which atoms or ions may be suitable candidates for qubits based on their electron configuration.
    a. Example: The Group I elements (Lithium, Sodium, Rubidium, Cesium) are often used because they have a single valence electron that can be used as a qubit.
    b. Example: The Group II elements (Calcium, Strontium, Barium) are often used as qubits when ionized (a single electron is removed), since that leaves them with a single remaining valence electron.

5. ENTANGLEMENT

Key Concept:

Entanglement, an inseparable relationship between multiple qubits, is a key property of quantum systems necessary for obtaining a quantum advantage in most QIS applications.

- When multiple quantum systems in superposition are entangled, their measurement outcomes are correlated. Entanglement can cause correlations that are different from what is possible in a classical system.
- An entangled quantum system of multiple qubits cannot be described solely by specifying an individual quantum state for each qubit.
- Quantum technologies rely on entanglement in different ways. When a fragile entangled state is maintained, a computational advantage can be realized. The extreme sensitivity of entangled states, however, can enhance sensing and communication.

Summary Description: Two or more quantum systems (for example, electrons or atoms) are entangled if their quantum states cannot be expressed independently. The added complexity of entangled states provides an advantage for quantum computing and sensing technologies.

Expectation: Students will be able to provide examples of how multiple atoms or electrons can be entangled with one another and produce measurement outcomes that cannot be explained by examining each part of the system independently.

Learner Outcomes

1. Students will describe how systems of many atoms or electrons can exist in quantum states that require understanding the system as a whole rather than as a collection of smaller parts.
    a. Example: In a Helium atom's ground state, the electrons have opposite spin quantum numbers, as demanded by the Pauli exclusion principle. The spin of each electron is not determined before being measured, but if one is measured to be spin-up, the other will be spin-down. These electrons are entangled with one another, and cannot be described independently.
    b. Example: In a water molecule, there are many important configurations where we cannot disentangle the state of the hydrogen atoms from the oxygen atom. Their properties are dependent on one another.
    c. Example: Two qubits may be entangled such that each qubit will be measured as "0" or "1" randomly, but if one is measured to be "0" the other will always be measured to be "1" and vice-versa.

Entanglement will be discussed further in an applications context in the Quantum Computing Key Concept.

6. COHERENCE

Key Concept:
For quantum information applications to be successfully completed, fragile quantum states must be preserved, or kept **coherent**.

- Decoherence erodes superposition and entanglement through undesired interaction with the surrounding environment. Uncontrolled radiation, including light, vibration, heat, or magnetic fields, can all cause decoherence.
- Some types of qubits are inherently isolated, whereas others require carefully engineered materials to maintain their coherence.
- High decoherence rates limit the length and complexity of quantum computations; implementing methods that correct errors can mitigate this issue.

Summary Description: A coherent superposition is a linear combination of quantum states (orbitals), and decoherence is the process by which superposition and entanglement are degraded through undesired interaction with the surrounding environment.

Expectation: Students will be able to explain how, due to the challenges of maintaining coherence, quantum systems can be very vulnerable to error.

Learner Outcomes
1. Students will describe how a linear combination (coherent superposition) of orbitals results in a different quantum state than simply one orbital or the other.
    a. Example: Collectively, equivalent resonance structures represent a linear combination of single- and double-bonds. Experimental observations show that the bond length of each bond lies between that of a single- and double-bond in many molecules (e.g., benzene, nitrate ions), which is consistent with a linear combination.
    b. Example: Hybrid orbitals do not have the same shape as the fundamental orbitals they are linear combinations of. For example, in a carbon atom, the hybridized sp3 orbitals are a linear combination of the s and p orbitals, but the hybridized orbitals are a different shape than the “s” and “p” orbitals.
2. Students will describe how even small amounts of decoherence can destroy the quantum state of a qubit.
    a. Example: A valence electron excited to a higher energy state can eventually decay to other lower energy states, destroying the information encoded in the qubit. Therefore, any operations on the qubit must be done within the lifetime of the excitation.
    b. Example: A valence electron in the ground state, the excited state, or any coherent superposition state may be affected by outside factors, such as

light/photons that excite it to another state or thermal excitations from the surrounding environment.

c. Example: A classical bit can only be corrupted by a complete bit flip (which changes 0 to 1 and 1 to 0), since it can only be in the state "0" or "1." Since the state of a qubit can be a linear combination (superposition) of "0" and "1," a qubit can also be corrupted by a partial bit flip, which affects the superposition.

3. Students will identify, in broad terms, the challenges in creating low-error qubits.
    a. Example: A qubit must be protected from the environment to avoid unintended errors, yet connected to the environment to be initialized, manipulated, and measured. These often contradictory goals are a challenge in designing and constructing useful qubits.
        i. As a specific example, radiation (light) can interact with an atom, causing the quantum state of the system to change.
    b. Example: Isolating the qubits from the environment requires keeping them at incredibly cold temperatures, well below 1 K.
    c. Example: Errors (such as bit flips or partial bit flips) can corrupt the state of a qubit, resulting in information stored in the qubit being lost.
    d. Example: Quantum error correction techniques need to be developed to protect qubit states against decoherence.

7. QUANTUM COMPUTING

Key Concept:
Quantum computers, which use qubits and quantum operations, will solve certain complex computational problems more efficiently than classical computers**.**

- Qubits can represent information compactly; more information can be stored and processed using 100 qubits than with the largest conceivable classical supercomputer.
- Quantum data can be kept in a superposition of exponentially many classical states during processing, giving quantum computers a significant speed advantage for certain computations such as factoring large numbers (exponential speed-up) and performing searches (quadratic speed-up). However, there is no speed advantage for many other types of computations.
- A fault-tolerant quantum computer corrects all errors that occur during quantum computation, including those arising from decoherence, but error correction requires significantly more resources than the original computation.

<u>Summary Description:</u> Quantum computers, which use qubits and quantum operations, will solve specific difficult computational problems more efficiently than classical computers.

<u>Expectation:</u> Students will provide examples of computational advantages and limitations of quantum computing in chemistry.

<u>Learner Outcomes</u>

1. Students will describe the necessary components to build a quantum computer.
    a. Example: A quantum computer must consist of many qubits that can interact with each other (become entangled), be transformed into superposition states and be measured independently. The operation of the quantum computer must finish before decoherence destroys the computation.
    b. Example: A quantum computer requires qubits that can be set to a known initial state, and the computation and measurement must take place before the quantum states of the qubits decohere.
    c. Example: Both quantum and classical computers require input, memory, processing, and output.
2. Students will describe different physical systems that can be used to build quantum computing devices.
    a. Example: The energy states of a variety of atoms can be used as qubits. In these systems, atoms are isolated and manipulated with laser beams to process quantum information or simulate other quantum systems.

    b. Example: Qubits can be encoded in various quantum states of light. Optical elements, such as beam splitters, are used to process quantum information.
3. Students will describe, in broad terms, how a quantum computer could be used to simulate and learn about other quantum systems.
    a. Example: In order to calculate properties of a molecule (such as ground and excited state energies), we need to understand the quantum-mechanical interactions within and between atoms in the molecule. Today's computers are not built for understanding quantum mechanics, but a quantum computer can be engineered to follow the same rules as a molecule of interest and efficiently calculate information about that molecule.
    b. Example: Aside from hydrogen-like atoms, solving for the ground states of atoms and molecules using the Schrödinger equation is impossible to do exactly. Approximate numerical methods are possible, and future quantum devices could greatly increase our ability to carry out these calculations.
    c. Example: Molecules made of many atoms can exist in entangled states that are more complex than their individual atoms. The complexity of these entangled states grows dramatically as the size of the molecules increase, greatly increasing the computational resources needed to model them. Quantum computers that can simulate these systems are required to study larger molecules.
4. Students will be able to explain potential use cases for quantum computers, and their advantages and limitations relative to classical computers.
    a. Example: Quantum computers can be used to more efficiently solve problems in chemistry, such as finding the energies and structure of atoms and molecules, and have a range of potential applications in environmental science, medicine, materials science, cryptography, and agriculture.
    b. Example: Quantum computers are special-purpose machines that provide a computational speedup that varies depending on the problem that is being solved. They are not suitable for all computational problems and applications (for example, quantum computers have no advantage for performing addition), and the additional resources needed for quantum computation are only worthwhile if they provide a strong computational advantage.
    c. Example: Quantum computers require classical computers to control and program them, and can be used in a feedback loop with high-performance classical computing. These "hybrid algorithms" have potential usage in understanding molecular structure using near-term quantum computers.

8. QUANTUM COMMUNICATION

Key Concept:
Quantum communication uses entanglement or a transmission channel, such as optical fiber, to transfer quantum information between different locations.

- Quantum teleportation is a protocol that uses entanglement to destroy quantum information at one location and recreate it at a second site, without transferring physical qubits.
- Quantum cryptography enhances privacy based on quantum physics principles and cannot be circumvented. Due to the fragility of quantum systems, an eavesdropper's interloping measurement will almost always be detected.

Quantum communication is less relevant as a topic for high-school chemistry classes. However, quantum chemistry and atomic physics is essential to developing enabling technologies for quantum communication and quantum networks such as quantum memories and quantum repeaters.

9. QUANTUM SENSORS

Key Concept:
Quantum sensing uses quantum states to detect and measure physical properties with the highest precision allowed by quantum mechanics.

- The Heisenberg uncertainty principle describes a fundamental limit in simultaneously measuring two specific, separate attributes. “Squeezing” deliberately sacrifices the certainty of measuring one attribute in order to achieve higher precision in measuring the other attribute; for example, squeezing is used in LIGO to improve sensitivity to gravitational waves.
- Quantum sensors take advantage of the fact that physical qubits are extremely sensitive to their surroundings. The same fragility that leads to rapid decoherence enables precise sensors. Examples include magnetometers, single-photon detectors, and atomic clocks for improvements in medical imaging and navigation, position, and timing.
- Quantum sensing has vastly improved the precision and accuracy of measurements of fundamental constants, freeing the International System of Units from its dependence on one-of-a-kind artifacts. Measurement units are now defined through these fundamental constants, like the speed of light and Planck’s constant.

Summary Description: Quantum sensors use quantum states for detection and measurement with the highest precision allowed by quantum mechanics.

Expectation: Students will be able to provide examples of how quantum mechanics is applied in the development of real-world sensors.

Learner Outcomes

1. Students will describe how quantization (such as the discretization of energy levels) has been used to develop many sensing and measurement technologies.
    a. Example: Electron spin responds to electric and magnetic fields. The strength of the response changes depending on the material (e.g., types of human tissue), and is used in nuclear magnetic resonance (NMR) spectroscopy and magnetic resonance imaging (MRI) technologies.
    b. Example: Lasers are used in many sensing, communication, and computing technologies. Laser light is generated through stimulated emission, a process which starts by driving more electrons to the excited state than the ground state.
    c. Example: The precise transitions of electrons between orbitals in an atom correspond to light of a specific frequency, which is harnessed in atomic clocks to

    keep time with incredible accuracy. One second is currently defined as the time that elapses during 9,192,631,770 oscillations of the photons emitted from a Cesium-133 atomic clock.

2. Students will be able to identify how concepts from quantum information science can and have been applied to build new kinds of sensors.
    a. Example: Electron beam microscopes use the wave nature of free electrons to image with incredibly high precision, since their wavelength can be much smaller than that of visible light.
    b. Example: Bose-Einstein condensates are an exotic state of matter which cannot be described as a gas, liquid, or solid. This state of matter is very sensitive to magnetic fields and acceleration, and can be applied as a sensor to detect electromagnetic fields and gravity.
    c. Example: Diamonds are regular lattices of carbon atoms. When nitrogen impurities are present in the lattice, either naturally or during laboratory growth, this defect has a specific energy structure that is very sensitive to magnetic fields, allowing it to be used as a magnetic field sensor.

GLOSSARY TERMS

- **QUANTUM STATE**: The mathematical representation of the properties of a physical system, such as an atom.
- **WAVEFUNCTION**: A mathematical description of the quantum state, from which measurement probabilities can be calculated.
- **SUPERPOSITION**: A linear combination of quantum states. A superposition of atomic orbitals is known as a hybridized orbital.
- **BIT**: A binary digit (bit) is the smallest unit of information, which can take the value “0” or “1”.
- **QUBIT**: A quantum bit (qubit) is the smallest unit of quantum information, which can be in the quantum state “0” or “1” or a linear combination of them.
- **ENTANGLEMENT**: An inseparable relationship that can exist between quantum objects or qubits.
- **DECOHERENCE**: The process by which superposition and entangled quantum states are corrupted by interactions with the surrounding environment.
- **CLASSICAL COMPUTER**: A device that processes information by performing operations on bits. This term generally refers to the traditional computers used today.
- **QUANTUM COMPUTER**: A device that processes quantum information by performing operations on quantum bits (qubits).
- **SENSOR**: A device or process that provides information about the state of an object or the environment (e.g., a magnetic field).

Below, you will find a summary of the topics in the QIS framework, along with keywords drawn from the American Association of Chemistry Teachers (AACT) activities and potential links to the Next Generation Science Standards (NGSS). Please note that the AACT keywords and links to NGSS are forward-looking and meant to serve as conversation starters for the development of curricular activities. This framework is an invitation for collaboration between educators and researchers for developing these curricular activities and lesson plans.

QIS Topic / Concept	**Short description**	**QIS Key Concept Section**	**AACT Subtopics**	**Extra Keywords**	**NGSS**
Quantum information science	Overview of field	1.0	Interdisciplinary, Scientific Method		HS-ETS1-1
Quantum state	Distinct quantum states	2.1	Bohr Model, Electron configuration, Orbitals, Quantum Numbers	Spin	HS-PS1-1 HS-PS4-3
	Quantization	2.2	Bohr Model, Orbitals, Quantum Numbers	Discretization	HS-PS4-3
	Evidence for quantization	2.3	Atomic Spectra, Atoms, Electrons, Emission Spectrum, Observations, Scientific method	Photons	HS-PS4-1 HS-PS4-3
	Electronic transitions	2.4	Atomic Spectra, Emission Spectrum	Excitation, Photon absorption	HS-PS4-1 HS-PS4-4 HS-PS4-5
	Superpositions / Linear combinations	2.5	Orbitals, Molecular Shapes, Resonance	Hybridization	HS-PS2-6
Quantum	Probability	3.1	Model of the	Probability	HS-PS4-3

measurement	distributions		Atom, Orbitals, Molecular shapes		
	Measurement tools	3.2	Emission spectrum	Magnetic resonance (NMR)	HS-PS4-4 HS-PS4-5
	Measurement statistics	3.3	Emission spectrum, Inferences, Observations, Model of the Atom, Orbitals, Molecular shapes	Probability	HS-PS4-5
Qubits	Binary information	4.1			MS-PS4-3 HS-PS4-2
	Encoding qubits	4.2	Atoms, Model of the Atom, Orbitals, Quantum numbers, Valence electrons	Spin	HS-PS1-1
	Qubits vs. classical bits	4.3	Atomic theory	Hybridization, Probability	MS-ETS1-2 HS-PS4-2
	Controlling qubits	4.4	Electron configuration, Orbitals, Valence electrons	Excitations	HS-PS4-4 HS-PS4-5
	Measuring qubits	4.5	Emission spectrum, Experimental design, Identifying an Unknown, Inferences	Probability	HS-PS4-4 HS-PS4-5
	Choosing qubits	4.6	Atoms, Ions, Elements, Periodic Table,	Spin	MS-ETS1-2 HS-PS1-1 HS-ETS1-3

			Trends of the Periodic Table, Valence electrons		
Entanglement	Entangled states	5.1	Electron configuration, Molecular structure, Measurements	Pauli exclusion principle	HS-PS2-6
Coherence	Superpositions / Linear combinations	6.1	Orbitals, Molecular Shapes, Resonance	Hybridization	HS-PS2-6
	Decoherence	6.2	Valence electrons, Radiation, Temperature		HS-PS4-5
	Challenges of making qubits	6.3	Error Analysis, Experimental design, Radiation, Temperature		HS-ETS1-2 HS-ETS1-3
Quantum computing	Components of quantum computers	7.1	Experimental design		MS-ETS1-3 HS-ETS1-2 HS-ETS1-3
	Physical systems	7.2	Atoms, Ions, Electrons, Valence Electrons, Trends in the Periodic Table	Photons, Spin	MS-ETS1-2 HS-PS1-1 HS-PS4-3 HS-ETS1-2
	Quantum simulation	7.3	Chemical structure, Molecular structure		MS-PS1-1 MS-PS1-3 MS-ETS1-2 HS-ETS1-2 HS-ETS1-3
	Uses for quantum computing	7.4	Chemical structure, Molecular		MS-PS1-3 MS-ETS1-1 MS-ETS1-2

			structure, Interdisciplinary		HS-ETS1-1 HS-ETS1-2 HS-ETS1-3 HS-ETS1-4
Quantum sensors	Quantum sensors today	9.1	Identifying an unknown, Measurements, SI Units, Accuracy, Orbitals	Lasers, Magnetic resonance, Atomic clocks	MS-ETS1-3 HS-PS4-4 HS-ETS1-2 HS-ETS1-3
	Quantum information enabled sensors	9.2	Identifying an unknown, Measurements, Phase Changes, Accuracy, Electrons		MS-ETS1-3 HS-ETS1-2 HS-ETS1-3

Examples of Chemistry Crosscutting Themes

Regarding connections to NGSS, the working group drafted cross-cutting theme information specific to quantum information science https://ngss.nsta.org/crosscuttingconceptsfull.aspx. Below, each NGSS cross-cutting theme is listed. The blue text is the output from the working group related to each theme.

1. Patterns:
Observed patterns in nature guide organization and classification and prompt questions about relationships and causes underlying them.
(a) A pattern that occurs across many quantum systems is that they can only exist in a discrete (quantized) set of states, such as many atomic energy levels (orbitals) and electron spin states.
(b) A pattern among quantum programs is that they use features like superposition (linear combinations) and entanglement, distinguishing them from their classical equivalents.
(c) Patterns that are similar among both classical and quantum computers are that they must be able to:

- Encode information in a physical system
- Initialize the physical systems
- Transform the information
- Measure the information as an output or result

(d) Patterns that differ between classical and quantum bits are that:

- Qubits are fragile, while classical bits are robust
- Classical bits have a definite state, but qubits can be in a superposition (linear combination) state with different measurement probabilities
- Classical bits can be described individually, while quantum bits can be entangled with each other

These differences in patterns are leveraged in technologies such as quantum computing and quantum key distribution.

2. Cause and effect:
Events have causes, sometimes simple, sometimes multifaceted. Deciphering causal relationships, and the mechanisms by which they are mediated, is a major activity of science and engineering.
(a) If we change the state of a qubit to a superposition (linear combination) state, the probability of measuring certain outcomes may change. **The cause is the preparation of the qubit in a superposition state, and the effect is a change of the measurement outcome probabilities.**
(b) If two qubits are entangled, their measurement outcomes may be correlated. **The cause is entanglement, and the effect is correlated measurement outcomes.**

3. Scale, proportion and quantity:

In considering phenomena, it is critical to recognize what is relevant at different size, time, and energy scales, and to recognize proportional relationships between different quantities as scales change.
(a) Quantum systems are typically much smaller than classical systems. For example, the typical size of an atom is 10^{-10} meters.
(b) The standard units of time are defined in relation to fundamental quantum quantities, which describe behavior at the sub-microscopic scale. The SI unit of time (the second) is defined relative to the Cesium-133 atomic clock transition.
(c) The advantage that quantum computers can have over classical computers grows as the size and depth of the quantum system increases. One of the principal challenges of quantum computing is engineering systems containing many qubits, as sources of error such as decoherence become more difficult for larger systems.

4. Systems and models:
A system is an organized group of related objects or components; models can be used for understanding and predicting the behavior of systems.
(a) The properties of electrons in an atom can be complex, but can be modeled with a discrete set of quantum numbers.
(b) Many quantum systems can be modeled as qubits, including:
- The energy states of atoms
- The spin states of electrons

5. Energy and Matter
Tracking energy and matter flows, into, out of, and within systems helps one understand their system's behavior.
(a) Over the course of a quantum computation, qubits will transition between different quantum states and superpositions (linear combinations). In many qubit implementations, this is realized by transitioning between different energy levels (orbitals).
(b) When electrons transition from a higher energy to a lower energy, they emit energy in the form of light (radiation), resulting in a particular emission spectrum.
(c) Qubits are surrounded by an environment, including other matter and stray energy such as light (radiation). Decoherence results when the qubits interact with this environment, and is the main reason qubits are exceptionally fragile.

6. Structure and Function:
The way an object is shaped or structured determines many of its properties and functions.
(a) An electron in a superposition (linear combination) state has a distinct orbital shape depending on the orbitals that make up the superposition.
(b) When considering the probability of measuring a certain outcome, we must consider both the quantum state and the type of quantum measurement.
(c) Quantum programs are structured to use features like superposition and entanglement. The function of this is to obtain the correct answer to a problem with high probability. This can result

in a computational advantage over classical programs in problems such as optimization and chemical structure simulation.

7. Stability and Change:

For both designed and natural systems, conditions that affect stability and factors that control rates of change are critical elements to consider and understand.

(a) Quantum states are fragile. The quantum states can change uncontrollably due to unwanted interaction with the environment, such as radiation.

(b) To reduce decoherence in a quantum computer, the system is maintained at a very low temperature. Quantum error correction techniques must be developed to protect against decoherence.

(c) Controlling the state of a qubit requires understanding what inputs it responds to. For example, a laser beam with the right frequency can flip the state of a qubit encoded in the valence electron of a trapped atom.