VISITING SCHOLAR PROGRAM

The PHI BETA KAPPA Society

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Public Lecture Offerings

Molecules and light: A story of life, death, and our quest for knowledge

Interactions between molecules and light are essential to life on Earth. They play a key role in the natural and artificial harvesting of solar energy that powers our planet. On the other hand, light can damage living organisms and materials by producing reactive open-shell species. Interactions between molecules and light enable us to study the world around us, whether we are using ordinary visual perception to see objects on a macroscopic scale, spectroscopy to examine objects on a microscopic scale or far out in space, or interrogating processes in live organisms with atomic-level resolution. This lecture will discuss molecular-level picture of light-induced processes and highlight the role of computational chemistry in developing better bioimaging probes.

This lecture is suitable for a general science-interested audience (at the Scientific American level). I delivered such a lecture as a Telluride town talk, where it generated much interest and lively discussions

The magic of of bioimaging: Spying on the molecules inside us

How can we see what is happening on a molecular level, in real time, inside living organisms? Can we see features smaller than the fundamental limit imposed by quantum mechanics? Genetically encoded fluorescent labels, derived from a fluorescent protein found in a jelly fish, have revolutionized our ability to observe fundamental process inside cells, with molecular resolution. These techniques, which have been recognized by two Nobel prizes, continue to deliver more fascinating possibilities. This lecture will explain the key ideas behind bioimaging, illustrating its power by examples, and reveal the connections between bioimaging and quantum mechanics.

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Classroom Discussion Topics

Chemistry with computers: Past, present, and future

Quantum mechanics provides a complete description of chemistry, biology, and materials. By simply specifying the particles (nuclei and electrons), we can write the Hamiltonian and the time-dependent Schrödinger equation, whose solutions define any imaginable physical property of the system. This is a truly amazing achievement of theoretical physics and a major milestone of human innovation! Unfortunately, in between the initial knowledge of the interacting particles and the macroscopic physical properties of the system lies an object of an enormous complexity: the unknown manybody wave-function determined by the Schrödinger equation. The exact wave-function is exponentially complex because of the quantum entanglement between the particles; this translates to a huge size of the wave-function and prohibitive costs of solving the exact equations. Both the size of the wave function and the cost of solving the equations scale factorially with the system size, giving rise to the so-called curse of dimensionality. How then can one use quantum mechanics to answer practical questions? This lecture will discuss how quantum chemistry has been addressing this intimidating problem by developing mathematically rigorous hierarchies of approximations, with well-defined error bars. What exactly is quantum chemistry? How much of it is physics, mathematics, and computer science? This discussion will cover old and new strategies of taming the complexity of wave-function, including emerging connections between quantum chemistry, artificial intelligence, and quantum information science. The potential of quantum computing to overcome the curse of dimensionality will also be discussed.

Appropriate for science majors, can be part of both upper division classes and freshmen courses (e.g., advanced general chemistry).

The quantum chemistry behind bioimaging

The molecular-level picture of modern microscopies using fluorescent labels (such as Green Fluorescent Protein) will be discussed. Examples will illustrate how practical goals (e.g., manipulating colors, optical output, and photostability) are related to basic quantum mechanical concepts (molecular orbitals, fluorescence, radiationless relaxation, and photochemistry).

Appropriate for an undergraduate physical chemistry class or for advanced general chemistry, physics, or biochemistry freshmen course.

Spin in chemistry: What is a spin and why do we care about it?

The conversation can start with a brief overview of the quantum-mechanical description of electron spin and then focus on its role in chemistry, from the periodic table to magnetism, and important technologies (solar energy, OLEDs, quantum information science, etc.).

Appropriate for an upper division undergraduate class (chemistry or physics majors).