

# Pitt's 'quantum repository' to make learning chemistry easier

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Remember constructing ball-and-stick models of molecules in your high school or college chemistry classes? Well, that might soon be a thing of the past for Pitt students looking to get a three-dimensional understanding of molecular structures.

University of Pittsburgh chemists Geoffrey Hutchison and Daniel Lambrecht recently received a 2014 Camille and Henry Dreyfus Special Grant Program in the Chemical Sciences award for their project, "Creating an Open Quantum Chemistry Repository." This effort aims to create an open mobile-ready, web-based database of accurate, quantum calculations of [molecules](#). The "Pitt Quantum Repository" will consist at first of 50,000 to 100,000 molecules and quantum chemical data. The database will grow over time to include more molecules and more computed properties.

"It's [chemistry](#) in the 'cloud,'" says Hutchison, associate professor of chemistry in the University of Pittsburgh's Kenneth P. Dietrich School of Arts and Sciences.

Almost all areas of chemistry rely on the three-dimensional nature of molecules, including stereochemistry, symmetry, molecular interactions, and reactivity. Consequently, understanding and developing intuition of molecular geometry, distances, and dynamics are critical for students.

Yet topics such as chirality or basic shapes can be difficult to understand with the traditional two-dimensional depictions used in textbooks or

PowerPoint slides and handouts. At the same time, students are immersed in digital media with interactive 3D worlds of computer games and mobile devices, and they have high expectations of ubiquitous and readily accessible online resources. While many online chemistry databases offer 3D molecular shapes, few are interactive, comprehensive, well curated and maintained, user friendly, and mobile ready.

The Pitt Quantum Repository will allow instructors to put "QR" barcodes on handouts or presentation slides. Students will then be able to scan the codes during a lecture, taking them to an interactive 3D visualization on their phone or tablet.

"We may be incorporating [the "quantum repository"] in some lab manuals next spring," says Lambrecht, Pitt assistant professor of chemistry. "We want to start with the large lecture classes for greatest impact."

Provided by University of Pittsburgh

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