A new computer program simulates the important process of photoexcitation

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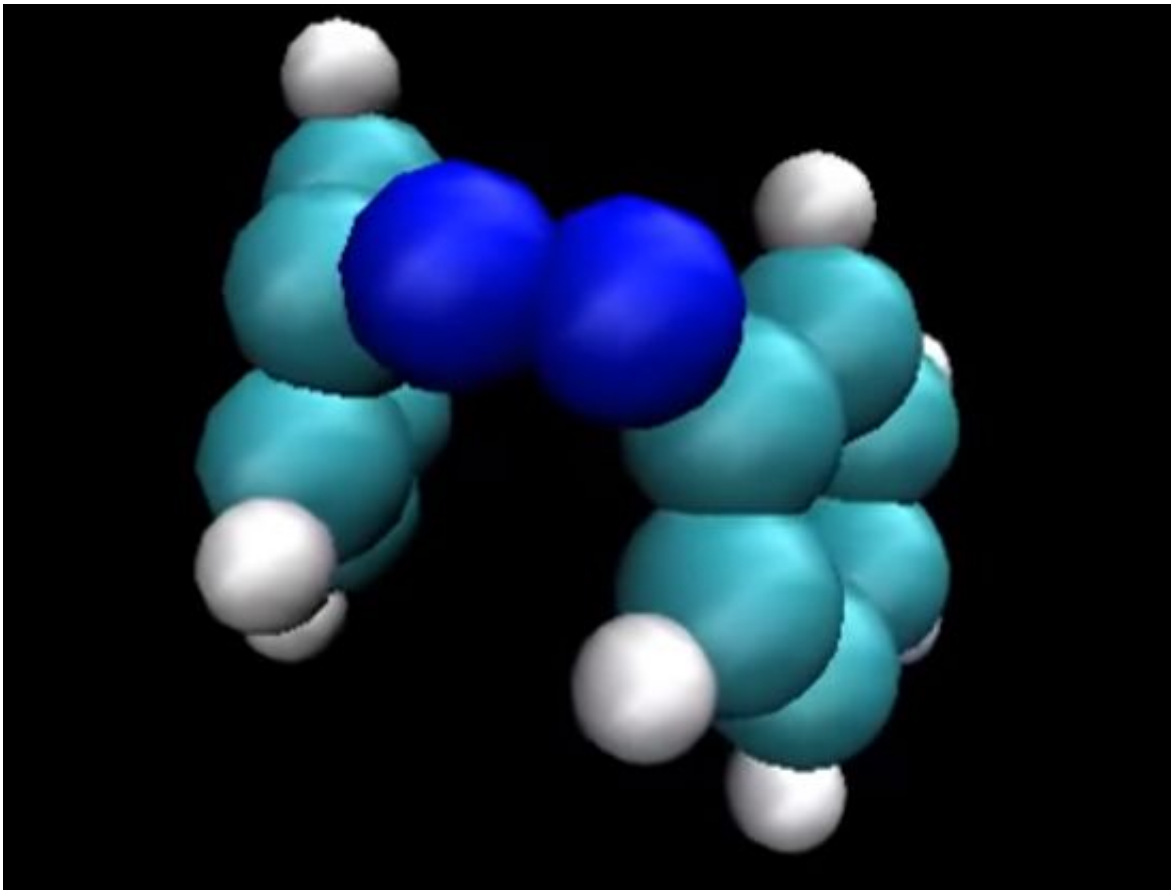

Photoexcitation is an important process in chemistry. It's what happens when a chemical compound absorbs light and enters an "excited" state in which the material has a higher electronic energy.

The process can help convert solar energy into usable electricity, or drive molecular machines whose parts rotate when an infusion of light prompts the molecules to change shape.

To propel these and other technologies forward, a University at Buffalo researcher has developed a new tool for studying photoexcitation: a computer program called Libra.

The open-source software gives scientists the building blocks to design their own algorithms for studying how a material or electronic state evolves over time. Among the program's capabilities: simulating what happens over time when a specific material is exposed to light.

Photoexcitation can alter molecules in ways that are invisible to microscopes, but important to understand. These changes, which can sometimes cause molecules to behave differently or adjust their shape, can be modeled using algorithms designed through Libra.

"Libra gives researchers a way to study the properties of many novel materials without having to fabricate each one experimentally," said the program's developer, Alexey Akimov, an assistant professor of chemistry in the UB College of Arts and Sciences. "This helps save time and money, as it takes resources to synthesize new materials in the lab."

So if a scientist is trying to build a molecular machine with a propeller that moves in a certain direction when exposed to light, he or she could use Libra to identify the molecular structures most likely to perform this task efficiently before deciding which structures to actually create in experiments.

Libra's capabilities are described in an article published on March 26, in the *Journal of Computational Chemistry*.

More information: Alexey V. Akimov. Libra: An open-Source "methodology discovery" library for quantum and classical dynamics simulations, *Journal of Computational Chemistry* (2016). DOI: 10.1002/jcc.24367