Slow-Motion Cameras for Chemical Reactions

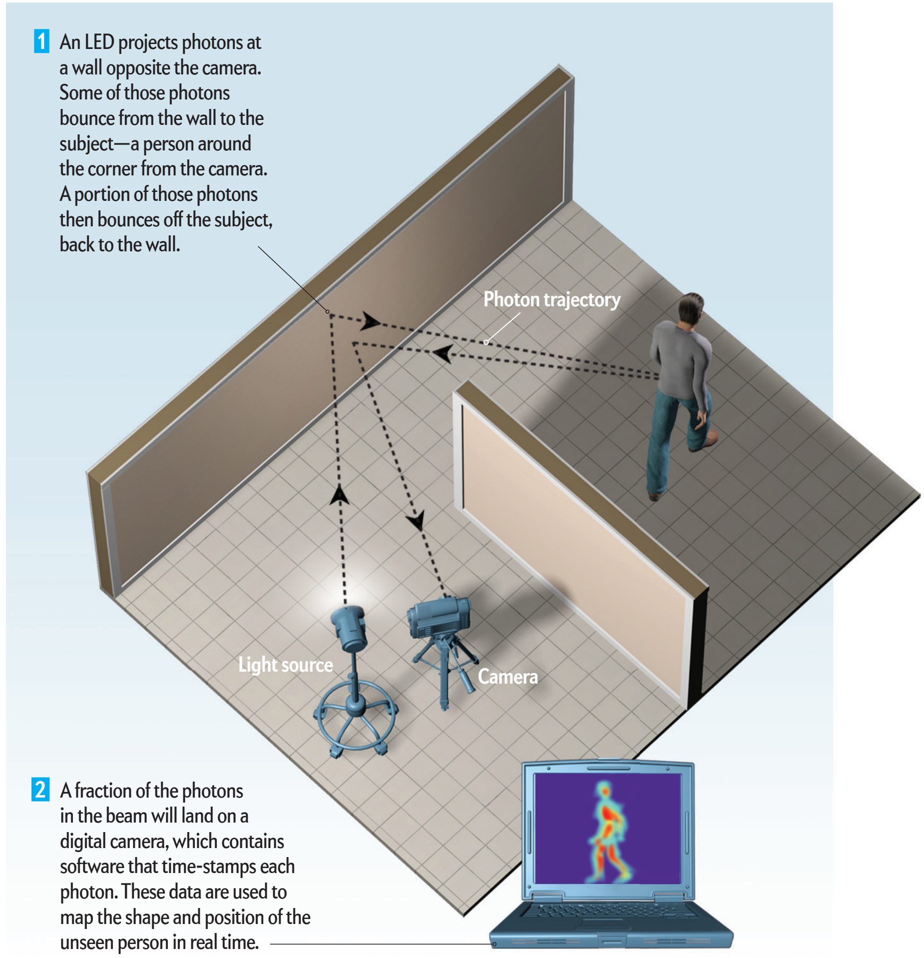
Infrared spectroscopy and computer simulations reveal the hidden world of solvent-solute interactions

The hydrogen bonds that hold together the molecular base pairs of our DNA form in intracellular fluid. Much of our planet's environmental chemistry occurs in oceans and other bodies of water. Most drugs are synthesized in solvents. Yet chemists generally study the bond-by-bond mechanics of chemical reactions only in the gas phase, where molecules are relatively sparse and easy to track. In a liquid there are more molecules and more collisions among them, so reactions are fast, messy and complicated. The process you want to observe will look like an undifferentiated blur—unless, that is, you can take snapshots of the reaction in a few trillionths of a second.

Andrew Orr-Ewing, a chemist at the University of Bristol in England, uses lasers to study chemical reactions. He knew that reactions in liquid catalyzed by heat create vibrations that can be observed in the infrared spectrum. In experiments conducted between 2012 and 2014, Orr-Ewing and then Bristol doctoral student Greg Dunning shot an ultrafast ultraviolet pulse at xenon difluoride molecules in a solvent called acetonitrile. The laser pulse acted like a scalpel, carving off highly reactive fluorine atoms, which in turn stole deuterium atoms from the solvent molecules, forming deuterium fluoride. The speed with which the telltale infrared vibrations appeared and then vanished after the first laser pulse—observed using a standard technique called infrared spectroscopy—revealed how quickly bonds formed between atoms and how quickly the reaction reached equilibrium.

The experiments were a proof of concept for observing the split-picosecond details of reactions in liquids. Most chemists, however, use computer simulations to observe and refine chemical reactions instead of expensive lasers and detectors. For them, Orr-Ewing's Bristol colleagues David Glowacki and Jeremy Harvey wrote simulation software that predicted the results of Orr-Ewing's spectroscopy experiments with an extraordinary level of accuracy. "We can use these simulations to peer more deeply into what's going on," Orr-Ewing says, "because they tell us more precise information than we can get from the experiments."

Together the experiments and simulations provide the best insights so far into how a chemical reaction actually happens in a liquid. Developers are already starting to incorporate the team's methods into computer simulations for academic and industrial use, which could benefit scientists doing disease research, drug development and ecological studies. —*J.A.*



Seeing around Corners

Bouncing photons let cameras see beyond the line of sight

If cameras could see around corners, they could warn drivers of danger waiting around the bend, help firefighters search burning buildings and enable surgeons to see hard-to-reach areas inside the body. A few years ago researchers at the Massachusetts Institute of Technology's Media Lab figured out how to build such a camera, but it was an expensive early prototype. The device used a laser pulse to bounce light from a wall or door onto a stationary object in the next room. A $500,000 camera then recorded the light that bounced back, and software recorded the arrival time of individual photons, calculated distances and reconstructed the unseen object. Since then, the M.I.T. team has improved the technology significantly. Now it can record moving objects beyond the line of sight, and instead of a laser and a $500,000 camera, an LED and a $100 Microsoft Kinect sensor will do. —*Larry Greenemeier*

Illustration by Don Foley