QnAs with Angel Rubio

Paul Gabrielsen, *Science Writer*

Just as physics requires a different set of tools to explore phenomena at the quantum scale, chemistry requires a quantum paradigm. At the macroscale, the interaction of light with chemical entities can be observed in processes such as photosynthesis. But the actual interaction between photons and other matter occurs in the realm of quantum chemistry. National Academy of Sciences member and physicist Angel Rubio, managing director of the Max Planck Institute for Structure and Dynamics in Hamburg, Germany, studies the theoretical interactions of photons and molecules in isolated cavities. Such cavities may be simple vacuums, or may contain mirrors that reflect particles within them at a frequency dependent on the cavities' dimensions. In his Inaugural Article (1), Rubio presents model systems of quantum chemistry that explore degrees of coupling between light and matter. Rubio recently spoke to PNAS about his findings.

PNAS: How does chemistry change at the quantum scale?

Rubio: When you put two atoms together, they form a chemical bond. Our players are molecules and photons. As there are two quantum entities, they will create a bond between the molecule and the photon field. This sort of quasi-particle is called a polariton. It's not an electron; not a photon. It's a mix.

PNAS: How do photons participate in chemical reactions?

Rubio: Our idea was to keep the normal chemical landscape, but add a new player that controls how these bonds are being formed or broken in the presence of this new glue between the atoms. This opens up what we call entangled chemistry. You might have heard of entangled physics, which is using quantum information theory to transfer information from A to B as fast as you can. You could use the same arguments now in chemistry. You can entangle molecules to be at a photon field to get the desired outcome of this reaction or this process. If you want to enhance energy transfer from a donor to an acceptor, you might put the donor–receptor [pairs] into a vacuum field such that these interactions are being mediated by the photon and enhanced. Or, if you want, you could quench it.

Angel Rubio. Image courtesy of Angel Rubio.

PNAS: What is the question that your Inaugural Article (1) is trying to address?

Rubio: We have new materials that when you put them in cavities—mirrors in which you incorporate either a molecule or a solid and drive the system out of equilibrium into a new state—they have properties that you could not get with the material in equilibrium. We decided, let's look to simple molecules and simple systems that we could solve exactly, and then show that you can really modify their properties and get something that is different to the way they behave in normal environmental conditions. Up to now, things

This is a QnAs with a recently elected member of the National Academy of Sciences to accompany the member's Inaugural Article on page 3026 in issue 12 of volume 114.

that had been done in solids were working at very low temperatures, below 4 Kelvin, which is interesting for fundamental physics, but is difficult to apply to real, technologically relevant materials in [real] life.

Many of these effects in atomic physics have been already explored. They used techniques of strong interactions between light and matter to bring atoms to low temperatures and then to enhance and be able to visualize quantum effects. We wanted to change the paradigm in which we work. We want to keep quantum phenomena alive at high temperatures.

PNAS: What role does light play in making high-temperature quantum effects possible?

Rubio: [Say] I put a molecule between two perfect reflecting mirrors. The length between the mirrors is such that this creates a wavelength with a frequency equal to the excitation of the molecule from the ground state to the first excited state, which is the absorption of light. In that particular case, the molecule is in a cavity in a complete vacuum. You don't even put light in. The properties of the molecule have been modified such that the molecule is completely different from a molecule in gas phase, without the mirrors. Then you see how you can modify that by adding external light sources to your system.

The beauty of this chemical phenomenon is that by having these molecules in cavities and many molecules interacting among themselves, these effects become robust, much larger than in the condensed phase until now, and can survive at room temperature. Now you can revisit what has been done in solids and materials, and then change the paradigm and make those effects visible at room temperature. This is what we plan to do in the future.

PNAS: What did you learn from examining the case studies in this paper (1)?

Rubio: We showed that we can change the bond length and vibrational frequency in the resonance of the cavity. Those are key elements in dictating chemical reactivity in realistic molecules with environments. We used different models, a dimer and a trimer, to illustrate that we can really control how the chemistry of those simple systems behaves in the cavity. And then we chose cases to show that in the resonant case we can get different results than in the nonresonant case. We can get higher efficiency of the process.

If we go to extremely high couplings, like matter couplings, then what we see is that the photon that goes through an atom is being absorbed and part of it remains attached to the atom. It's called the slowdown of photons by matter. Usually what happens is that the photon comes in, [gets] scattered, and immediately goes out.

The question now is: can we make use of those new states? This is the beauty of it; it allows you to unravel new quasiparticles. It's exciting because it's a new field with not too many players, but people are getting more and more interested in it.

1 Flick J, Ruggenthaler M, Appel H, Rubio A (2017) Atoms and molecules in cavities, from weak to strong coupling in quantum-electrodynamics (QED) chemistry. *Proc Natl Acad Sci USA* 114:3026–3034.