

What does mercury being liquid at room temperature have to do with Einstein's theory of relativity?

BY ASHUTOSH JOGALEKAR

This article was published in Scientific American's former blog network and reflects the views of the author, not necessarily those of Scientific American

One of the great moments in twentieth century science came when Paul Dirac married quantum mechanics with Einstein's Special Theory of Relativity to produce relativistic quantum mechanics. Dirac's theory did many things - predict electron spin and the positron, analyze atomic collisions, jump-start the revolution in [quantum electrodynamics](#) - but it also had very significant repercussions for chemistry. However these repercussions did not become known for another few decades because it turned out that for solving most problems in chemistry you could neglect relativistic effects. Figuring out chemical bonding, predicting the thermodynamic properties of molecules and rates of chemical reactions, understanding the molecular glue that holds proteins together; all these problems succumbed to calculation without chemists worrying about relativity.

All except one problem, that is. And it deals with a question that every child since antiquity has asked: Why is mercury liquid at room temperature? Mercury - the only metal with this property - has beguiled and fascinated men

for centuries; a glittering substance that flows with studied gravity, supports the weight of coins, magically seems to dissolve other metals and resists all attempts to scoop it up. A substance that can aid health when calibrated inside a thermometer and can kill when it accumulates in living tissues. But the one quality of mercury that is apparent to everyone who has even the slightest acquaintance with it is its liquid nature.

Why is this so? It turns out that sometimes simple observations in science can have complicated although very interesting explanations, and this is one of those cases. Fortunately the crux of the matter is simple, and it has received its most complete and satisfying treatment in a [recent paper](#) published in the journal *Angewandte Chemie*. But first let's go back to the basics. Mercury is a metal, which means that it occupies the middle of the periodic table along with other metals like gold, zinc and cadmium. In fact it is in the same group as zinc and cadmium, and yet it couldn't be more different from them. Zinc and cadmium are not liquids at room temperature and they crystallize in a different form from mercury. In addition mercury is right next to gold, and yet their properties are utterly dissimilar.

ON SUPPORTING SCIENCE JOURNALISM

If you're enjoying this article, consider supporting our award-winning journalism by [subscribing](#). By purchasing a subscription you are helping to ensure the future of impactful stories about the discoveries and ideas shaping our world today.

Recall from college chemistry that atomic orbitals come in different flavors; s, p, d and f orbitals are distinguished by different quantum numbers and different "shapes". Metals are characterized by significantly occupied d orbitals.

In addition, filled orbitals imply special stability. The singular fact that distinguishes mercury from its neighbors is that it has a filled outermost 6s atomic orbital. This means that the electrons in the orbital are happily paired up with each other and are reluctant to be shared among neighboring mercury atoms. Where the theory of relativity comes in is in accounting for subtle changes in the masses of the electrons in mercury and the atomic radii which nonetheless have profound effects on the physical properties of the metal. According to special relativity, the apparent mass of an object increases as its velocity approaches the speed of light. From Niels Bohr's theory of atomic structure we know that the velocity of an electron is proportional to the atomic number of an element. For light elements like hydrogen (atomic number 1) the velocity is insignificant compared to the speed of light so relativity can be essentially ignored. But for the 1s electron of mercury (atomic number 80) this effect becomes significant; the electron approaches about 58% of the speed of light, and its mass increases to 1.23 times its rest mass. Relativity has kicked in. Since the radius of an electron orbit in the Bohr theory (orbital to be precise) goes inversely as the mass, this mass increase results in a 23% decrease in the orbital radius. This shrinkage makes a world of difference since it results in stronger attraction between the nucleus and the electrons, and this effect translates to the outermost 6s orbital as well as to other orbitals. The effect is compounded by the more diffuse d and f orbitals insufficiently shielding the s electrons. Combined with the filled nature of the 6s orbital, the relativistic shrinkage makes mercury very reluctant indeed to share its outermost electrons and form strong bonds with other mercury atoms.

The bonding between mercury atoms in small clusters thus mainly results from weak Van der Waals forces which arise from local charge fluctuations in neighboring atoms rather than the sharing of electrons. But all this was conjecture; someone had to do the rigorous calculations, treating every

electron in the element relativistically and calculating the relevant properties.

In this case the relevant property is the heat capacity of a substance which dramatically changes during a phase transition, say from solid to liquid. The question was simple; using the most state-of-the-art calculations, could you predict the temperature at which mercury melts as indicated by a sudden change in heat capacity? In a paper published in *Angewandte Chemie* this month, chemists from New Zealand, Germany and France have provided a result which is the most complete one to date. They actually simulated the melting of mercury using quantum molecular dynamics, solving the Schrodinger equation, calculating forces and velocities from quantum mechanics and allowing the atomic clusters to sample different geometric orientations randomly. They carried out the calculations first by excluding relativity and then by including it, and the results were unambiguous; when relativistic effects were taken into account, the melting point of mercury dropped from 355 kelvin to 250 kelvin, in excellent agreement with experiment and accompanied by a sudden change in the heat capacity.

The liquid nature of mercury is not the only thing that the special theory explains. It also explains why gold is yellow while silver is white. In this case, the splitting of orbitals and the lower energy of the 6s orbital results in gold absorbing blue light and emitting yellow and red. Since the 6s level is higher in silver, the energy required to excite an electron corresponds to the UV region instead of the visible region; consequently silver appears devoid of colors from the visible region of the spectrum.

I always feel a twang of pleasure when I come across studies like this. There are few things more satisfying than the successful application of our most cherished and accurate theories to explaining life's most humdrum and yet fascinating phenomena. That's what science is about.

References:

1. Evidence for Low-Temperature Melting of Mercury owing to Relativity; F. Calvo et al. *Angew. Chem. Intl. Ed. Engl.* **2013**, 10.1002/anie.201302742
2. Why is Mercury Liquid? L. Norrby, *J. Chem. Ed.* **1991**, p. 110.
3. Relativistic Effects in Chemistry, D. McKelvey, *J. Chem. Ed.* **1983**, p. 112

[ASHUTOSH JOGALEKAR](#) is a chemist interested in the history, philosophy and sociology of science. He is fascinated by the logic of scientific discovery and by the interaction of science with public sentiments and policy. He blogs at The Curious Wavefunction and can be reached at curiouswavefunction@gmail.com.

More by [Ashutosh Jogalekar](#)

It's Time to Stand Up for Science

If you enjoyed this article, I'd like to ask for your support. *Scientific American* has served as an advocate for science and industry for 180 years, and right now may be the most critical moment in that two-century history.

I've been a *Scientific American* subscriber since I was 12 years old, and it helped shape the way I look at the world. *SciAm* always educates and delights me, and inspires a sense of awe for our vast, beautiful universe. I hope it does that for you, too.

If you [subscribe to *Scientific American*](#), you help ensure that our coverage is centered on meaningful research and discovery; that we have the resources to report on the decisions that threaten labs across the U.S.; and that we support both budding and working scientists at a time when the value of science itself too often goes unrecognized.

In return, you get essential news, [captivating podcasts](#), brilliant infographics, [can't-miss newsletters](#), must-watch videos, [challenging games](#), and the science world's best writing and reporting. You can even [gift someone a subscription](#).

There has never been a more important time for us to stand up and show why science matters. I hope you'll support us in that mission.



Thank you,
David M. Ewalt, Editor in Chief, *Scientific American*

[Subscribe](#)

Subscribe to *Scientific American* to learn and share the most exciting discoveries, innovations and ideas shaping our world today.

[Subscription Plans](#)

[Give a Gift Subscription](#)