Industrial Explosives

Ball estimates molecular energy to improve efficiency, greenness

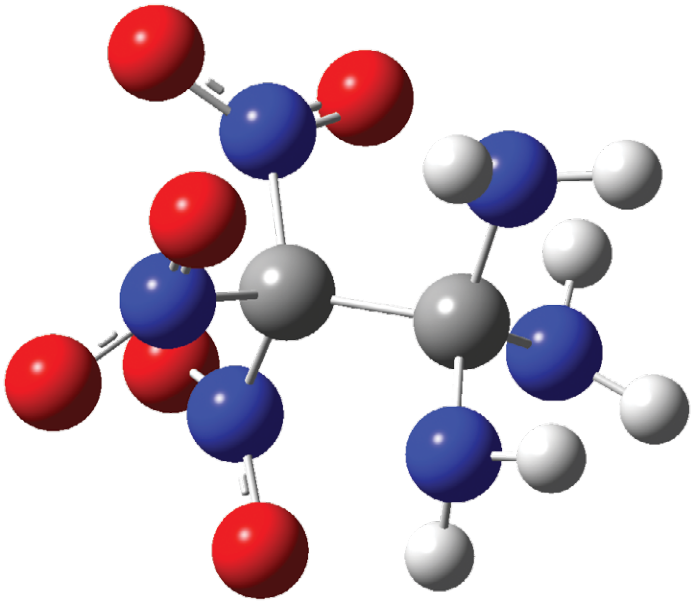
Alfred Nobel, namesake of the Nobel Prizes, was originally known for inventing dynamite, though not fondly, as he found out.

When his brother died, a newspaper erroneously reported Alfred's death. The obituary chided him for his invention that, especially at that time, often proved deadly. Afforded a rare glimpse of his potential legacy, the wealthy Nobel established the Prizes to ensure scholars are remembered for their positive contributions to society, as he wanted to be.

Over a century later, Cleveland State University's chair of the Department of Chemistry is working to ensure Nobel's invention is not only remembered, but continually improved. David Ball, Ph.D., is using OSC resources to calculate the thermodynamic properties of molecules for the application of new high energy density materials—or, put plainly, explosives.

"(OSC) is a great resource for the state of Ohio," Ball said. "It allows people who might normally not be able to have access to this kind of resource access to a modern computational facility where we can do cutting-edge work."

An explosion occurs when unstable molecules undergo a chemical reaction to create stable reaction products. In the case of high-nitrogen molecules, one reaction product is nitrogen gas, an energetically stable molecule. Other stable products include water and carbon dioxide. If a molecule has the right mix of carbon, hydrogen, oxygen and nitrogen, it can rearrange to create these stable products.



▶ Should it ever be synthesized, 1,1,1-triamino-2,2,2-trinitroethane (TTE) should give off 40 percent more energy than TNT, OSC-based calculations predict.

"In doing so, it gives off a lot of energy," Ball said. "That's where we get the energy from our fuels, that's where we get the energy from our explosives."

Explosives and similar fuels used for construction, military applications and as propellants give off huge amounts of energy when they decompose. Ball's group uses nodes on Oakley to estimate the energy of a given molecule and compare it to the energy of the decomposition products. The result is the amount of energy a molecule can potentially give off when it explodes.

The basic concepts of explosives are relatively simple; Ball and his students are evaluating the overall energy of these molecules in respect to possible reaction products to create more efficient, and possibly cleaner high energy density materials. Many products of these reactions are greenhouse gases. If the molecules can be rearranged into a product that's more efficient, not only will the fuels and explosives themselves be more useful in industry, but the environment as a whole will be better off as well—presumably what Nobel would have wanted. •

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