Scientists create a new electronegativity scale

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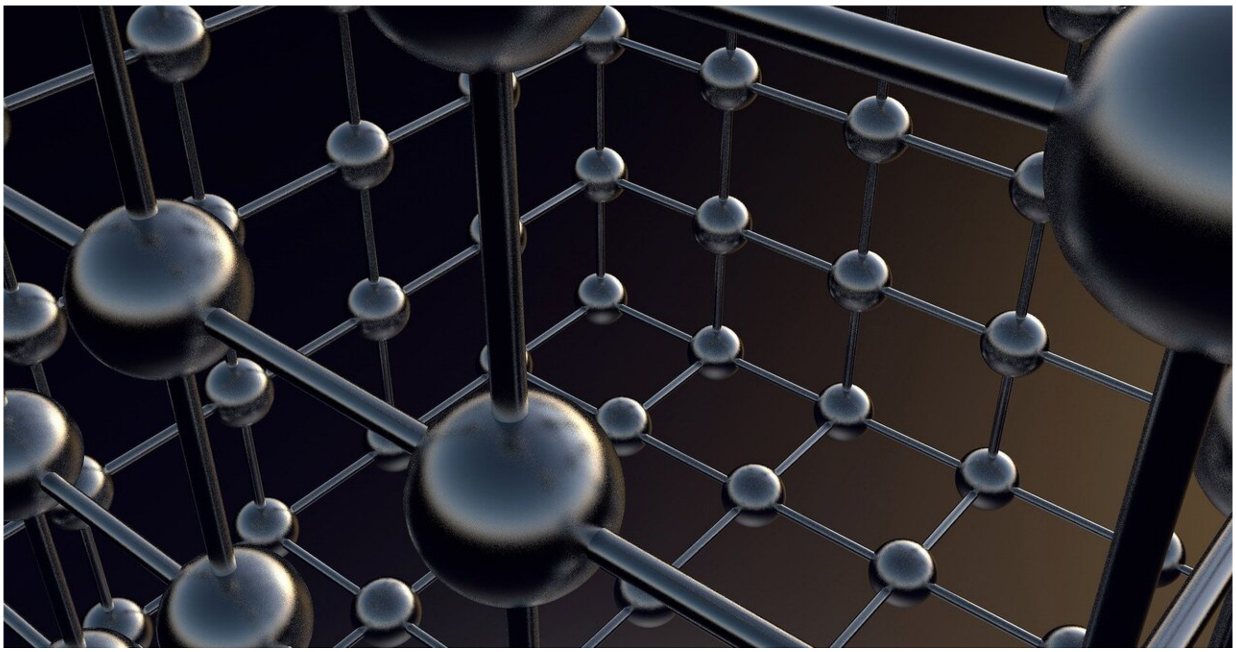

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Skoltech chemists have proposed a new electronegativity scale and published their findings in *Nature Communications*.

The concept of electronegativity introduced in the 1930s by Linus Pauling, a great American chemist, refers to the ability of an atom to attract electron density. In a chemical bond, the more electronegative atom gains extra electrons, becoming negatively charged, while the less electronegative one loses electrons and becomes positively charged.

Electronegativity is essential for explaining things that range from the energy of chemical bonds to the (in)stability of chemical compounds and the color and hardness of crystals.

Since then, chemists have come up with various definitions and scales of electronegativity. Yet Pauling's scale is the first and the most common one, present in every chemistry textbook. Pauling deduced his electronegativity values from thermochemistry using the energies of some chemical bonds. He proposed the simplest formula to calculate a bond's stabilization due to the difference in electronegativity between the atoms. It later transpired that the predictions made with Pauling's scale had a rather low accuracy.

Skoltech Professor Artem R. Oganov and research scientist Christian Tantardini ventured to modify Pauling's formula and redefine the electronegativities of elements and ended up creating a new scale of electronegativity.

"It all started when we decided to calculate Pauling's electronegativities under pressure. The chemistry of high pressures is quite exotic. Still, you will likely be able to understand a lot of things once you find out how the electronegativities of elements change under pressure. We used Pauling's definition to calculate electronegativity under normal conditions. We were amazed to discover that his scale did not match either theoretical or experimental bond energies for significantly ionic molecules. Moreover, many publications in chemical literature mention this inconsistency, but none offer a consistent solution. I realized that the root cause was that Pauling treated the molecule's ionic stabilization as an additive effect. If we consider it a multiplicative effect, many drawbacks will be removed. With the new formula and experimental energies of chemical bonds, we determined the electronegativities of all the elements. We obtained a beautiful scale that works both for small and large differences in electronegativity," Professor Oganov explains.

The new scale uses electronegativity as a dimensionless quantity, which is very practical and accurately reproduces both molecules' energies and chemical reactions.

More information: Christian Tantardini et al. Thermochemical electronegativities of the elements, *Nature Communications* (2021). DOI: 10.1038/s41467-021-22429-0

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