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Moving towards a predictive model for chemical phenomena

Dr. Eduardo Chamorro, full professor and researcher of the Chemistry Department of the Faculty of Exact Sciences at the Universidad Andrés Bello, is working on a research project to construct a mathematical model to predict chemical phenomena of different natures.

The UNAB investigator explains that, "The models that we construct could be applied to any type of chemical reaction, saving time and resources and acting as a valuable tool in complex scientific research."

As a first step, Dr. Chamorro indicates that a system needs to be designed to operate predictively. Existing information on chemical reactions and influencing factors is then imputed into this system. Following this, the system is then run through test simulations of reactions, and the results are contrasted against experimental data.

The final goal of this model, which is being developed with the support of the National Commission for Technological and Scientific Investigations (Conicyt), is to comprehensively understand reactions within the chemical systems of nuclei and electrons. This would include, for example, if energy increases or decreases.

To achieve this, the reactions are classified into three large categories, where global reactions affect the whole system; local reactions affect only part of the system; and delocalized reactions occur in one area of the system but affect another.

Finally, Dr. Eduardo Chamorro explains that, "Reality is far more complex than any theory, and we are constantly testing the system. Nevertheless, the idea is to implement a freely distributed, web-based software that could receive fundamental feedback from groups working on cutting-edge research."