

Expanding the range of nature's catalysts for industrial applications

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To make paper, manufacturers must break down cellulose (chunks of wood pulp), a process that currently requires large amounts of energy and toxic chemicals like chlorine. Nature performs the same task using enzymes, non-toxic biodegradable proteins that accelerate chemical reactions using far less energy. The catch is that the enzymes required for the job, in this case xylanases, don't hold up to the high temperatures of the manufacturing process. This is only one of many examples of how the limitations of enzymes hamper the development of elegant solutions in the manufacture of everything from medicine to detergents.

"So the question is: can we improve on nature?" said George Makhatadze, a chaired professor in the Biocomputation and Bioinformatics research constellation, professor of biological sciences, and member of the Center for Biotechnology and Interdisciplinary Studies (CBIS) at Rensselaer Polytechnic Institute. "Can we take an existing protein and, using computation, redesign it to withstand higher temperatures?"

Makhatadze designs "custom proteins," and is an expert in the critical interaction between electrical charges on the surface of proteins. Within the School of Science, Makhatadze's research is part of an interdisciplinary theme of modeling, analysis, and simulation. His research is also part of a CBIS research focus on [protein engineering](#). In a 2009 edition of the *Proceedings of the National Academy of Science* (PNAS), his lab presented a computer model that enhances protein thermostability, while retaining full enzymatic activity. Now, with the

support of a five-year, \$1.7 million National Science Foundation grant, Makhatadze will investigate the speed of [protein folding](#).

Enzymes are composed of long strings of amino acids. As the string is assembled, electrostatic forces along its length interact, causing it to twist and turn, and ultimately fold into a stable three-dimensional shape. The enzyme functions properly only when folded into this shape, and typically retains its structure within a narrow range of conditions. If subjected to temperature, pH, or pressure outside these tolerances, the enzyme begins to denature, losing its shape and functionality.

Makhatadze seeks to boost the high-temperature tolerances for a given enzyme by adjusting the electrostatic interactions on the [protein surface](#). In research culminating with the 2009 PNAS paper, Makhatadze developed a computer program allowing researchers to expand the temperature range at which a given enzyme would remain functional by altering the electrical charges on the protein surface.

"Many forces – the packing of the core, hydrophobic interactions, hydrogen bonding, salt bridges, disulfide bridges – are important for protein stability, and 40 years of research has gone into establishing the rules that govern this process," said Makhatadze. "Our contribution has been on the particular role of the interactions between the charges on the protein surface, and a recognition that they can be manipulated to modulate protein stability."

In the context of industrial processes like paper manufacturing, the expanded functional range could make an enzymatic approach more attractive and economically feasible. The next step, said Makhatadze, and the focus of the NSF grant, is to understand the speed at which proteins fold and unfold, in order to slow their deterioration, and further expand their functional range.

"We've learned to make changes in the stability of the protein. But every protein has a limit; there's nothing you can do to make a [protein](#) stable at 500 degrees, for example," said Makhatadze. "So can we somehow make it unfold more slowly by modulating the charge-charge interactions? If you can extend that process, it will function at a high temperature for a longer period of time, and that's beneficial."

Within CBIS, the \$1.7 million commitment from the NSF is one of several new multimillion-dollar research awards, raising research expenditures in 2014 despite a challenging funding environment.

Provided by Rensselaer Polytechnic Institute

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