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Autonomous Combinatorial Experimentation for Streamlined Materials Discovery

Machine learning has become an integral part of many aspects of materials research. As a branch of machine learning, active learning has attracted much attention recently, as it can effectively help navigate experimental sequences in materials research. We are incorporating active learning in combinatorial exploration of functional materials in autonomous modes. The array format with which samples of different compositions are laid out on combinatorial libraries is particularly conducive to active learning. Autonomous experimentation can be used to reduce the number of required experimental cycles by an order of magnitude or more. Using the closed-loop autonomous materials exploration and optimization (CAMEO) scheme, we have discovered a new phase change memory material which outperforms the industrial standard by a significant margin. I will also discuss other autonomous experimentation projects we are carrying out including implementation in neutron scattering, development of low-cost robot-science kits, and demonstration of real-time experiment-theory closed-loop interaction. This work is performed in collaboration with A. Gilad Kusne, H. Liang, L. Saar, A. McDannald, H. Yu, A. Mehta, and V. Stanev. This work is funded by NIST, SRC, ONR, and AFOSR.

Ichiro Takeuchi is a professor of materials science and engineering and affiliate professor of physics at the University of Maryland. He received his Ph.D. in physics from the University of Maryland in 1996. Prior to joining the University of Maryland faculty, he was a postdoctoral research associate at Lawrence Berkeley National Laboratory, where he helped pioneer the combinatorial materials synthesis strategy. Takeuchi's research program is focused on combinatorial exploration of novel functional materials, development of elastocaloric materials and systems, and superconducting devices. Since 2009, Takeuchi has also served as the CTO of Maryland Energy & Sensor Technologies, LLC, a start-up dedicated to development of elastocaloric cooling systems. Takeuchi is a fellow of the American Physical Society and the Japan Society of Applied Physics.

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