

differs depending on how much oxygen is in the blood, allowing the device to read blood-oxygen concentrations.

The device performed as well as previous organic pulse oximeters that use glass and thick plastic substrates, but had the added benefit of being ultrathin and being strongly adhesive. “Our device is very thin, so we can achieve [a] very stable signal,” Yokota says.

“The flexibility of organic semiconductors makes them a natural technology for

wearable sensors,” says Ifor Samuel of the Organic Semiconductor Optoelectronics Group at the University of St. Andrews, who was also not involved in the study. “This work shows a promising advance in flexible encapsulation of such devices.”

Dae-Hyeong Kim, a researcher in flexible electronics at Seoul National University, adds that the work is “extremely important” for the field of deformable optoelectronics used in long-term health monitoring due to the softness of

the device. As mobile electronics become more prevalent, “this technology would become one of [the] good technological solutions toward fully integrated wearable electronics and bioelectronics,” Kim says.

The researchers are now looking to fabricate a full-color e-skin display and further improve the stability of the device in air. “If we succeed [in improving] stability, we want to use our device in water,” Yokota says.

**Joseph Bennington-Castro**

### Adaptive design loop ushers exploration of new materials

Advanced materials discovery is essential to economic security, technological advance, and social welfare. However, it often takes a few decades from initial discovery to market due to challenges in finding the optimal materials properties for certain applications. The enormous degree of complexity in manipulating materials properties comes with countless “knobs” to turn when designing the experimental approach. Strategies are needed for a design-feedback loop to locally exploit and globally explore optimized solution from hundreds of thousands of possible candidates. The adaptive design loop incorporates statistical inference, machine learning, design, and experimental feedback to optimally guide future experiments. The loop is finding relevance in materials design ranging from metal alloys to polymers, ceramics or nanomaterials, where researchers are searching for target materials properties.

In a recent issue of *Nature Communications* (doi:10.1038/ncomms11241), a research team, led by Turab Lookman in the Theoretical Division at Los Alamos National Laboratory, developed a data-driven framework to effectively navigate new materials discovery with targeted property optimization. “The key question we addressed is the following: how do we optimally guide the next experiment(s) or calculation(s), in search of materials with a desired response,

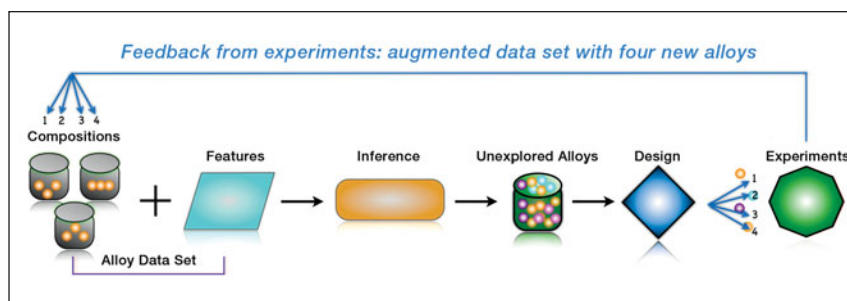


Illustration of adaptive design loop experiment of NiTi-based alloy system. Credit: Turab Lookman.

especially when the search space is vast?” Lookman says. The answer is to incorporate uncertainties in designing the experiments. The predicted data points with larger uncertainties will facilitate greater exploration in global search, even when the mean predicted values are far from desired. In contrast, the predicted data points with smaller uncertainties favor exploitation in local search.

The strategy was used to find very low thermal hysteresis ( $\Delta T$ ) in NiTi-based shape memory alloys with nearly 800,000 potential alloys in the  $\text{Ni}_{50-x-y-z}\text{Ti}_{50}\text{Cu}_x\text{Fe}_y\text{Pd}_z$  family to choose from. The demonstrated adaptive design loop starts with collecting prior knowledge of 22 initial alloys with measured materials properties. Statistical models are used to predict materials properties and suggest new experiments. On the sixth of nine iterations of the adaptive design loop, an alloy with the lowest  $\Delta T$  was discovered at an optimized materials composition. In each iteration, four alloy compositions were predicted and

synthesized. Fourteen out of 36 alloy compositions were found to have  $\Delta T$  smaller than the best data points in the original data set. “A key component of our strategy is ‘design,’ recommending the next experiments to be performed in order to improve subsequent model predictions, hence adaptive design,” Lookman says.

“This type of approach brings the best statistical ideas to materials discovery and design. While the methods have seen substantial use in genomics and machine learning, their use in materials research opens the door to better targeted experiments; improved materials models; and a deeper, more effective science of materials,” says James A. Warren, the director of the Materials Genome Program at the National Institute of Standards and Technology. “These methods, and their successors, will accelerate new materials-into-application, finding use across the breadth of materials research.”

**YuHao Liu**