Discovering New Molecules for Military Applications

AI chemistry program aims to accelerate creation of novel, high-performance molecules for defense needs

outreach@darpa.mil

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The efficient discovery and production of new molecules is essential for a range of military capabilities—from developing safe chemical warfare agent simulants and medicines to counter emerging threats, to coatings, dyes, and specialty fuels for advanced performance. Current approaches to develop molecules for specific applications, however, are intuition-driven, mired in slow iterative design and test cycles, and ultimately limited by the specific molecular expertise of the chemist who has to test each candidate molecule by hand.

Today, DARPA announced the Accelerated Molecular Discovery (AMD) program, which aims to develop new, AI-based systematic approaches that increase the pace of discovery and optimization of high-performance molecules. A Proposers Day webinar describing the goals of the program is scheduled for Oct.18, 2018. Details are available here: https://go.usa.gov/xPk5j

"The ultimate goal of AMD is to speed the time to design, validate, and optimize new molecules with defined properties from several years to a few months, or even several weeks," said Anne Fischer, program manager in DARPA's Defense Sciences Office. "We aim to develop the AI tools, models and experimental systems to enable autonomous design of molecules to quickly meet DoD needs."

The program calls for teams of researchers to develop AI-based, closed-loop systems that automatically extract existing chemistry data from databases and text, perform autonomous experimental measurement and optimization, and use computational approaches to develop physics-based representations and predictive tools.

AMD performers will develop tools, models, and experimental capabilities to rapidly design, validate, and optimize molecules. Government partners will evaluate performer developments and test their ability to identify new molecules with specific combinations of functional properties that may be relevant to specific DoD application requirements.

"There are currently around 140 million known molecules, but the space of potential molecules is vastly larger than that, upwards of 10^{60}," Fischer said. "In DARPA's Make-It program, we've developed advanced ways to efficiently synthesize known molecules. AMD is taking the next step, where we will rapidly be able to explore the unknown molecular universe to design and produce completely new molecules with specific desired functions."

The AMD program seeks expertise in chemistry and chemical engineering, computer science, AI/machine learning, and mathematics. A Broad Agency Announcement (BAA) solicitation with full details is expected to be published soon on FedBizOpps here: http://go.usa.gov/3W53j

Image Caption: *DARPA's Accelerated Molecular Discovery (AMD) program aims to develop new, AI-based systematic approaches that increase the pace of discovery and optimization of high-performance molecules.*

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