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TECHNION - ISRAEL INSTITUTE OF TECHNOLOGY

הפקולטה להנדסה כימית
ע״ש וולפסון
The Wolfson Department of Chemical Engineering

Wolfson Department of Chemical Engineering Seminar

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Room 6

Developing a Generative Search Tool for Novel Energetic Materials

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MSc Seminar

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Energetic materials, the explosives and propellants underlying applications from mining and demolition to defense, must deliver high performance while remaining safe to handle. Discovering new ones is slow and hazardous: the chemical space is enormous, experimental testing is costly and dangerous, and a fundamental trade-off between energy and sensitivity constrains every candidate. Computational design promises to accelerate this search, but existing methods rarely consider whether a proposed molecule can actually be synthesized, so their candidates are frequently impossible to make in the laboratory.

In this seminar, I will present a generative framework that designs new energetic molecules together with a model that judges whether those molecules can actually be made. The framework follows a four-stage pipeline: a physics-constrained genetic algorithm assembles a library of energetically relevant molecules; a novel variational autoencoder learns a continuous map of chemical space in which properties can be predicted and navigated; multi-objective optimization searches this space for the most promising candidates; and density functional theory validates the top designs. Because standard synthesizability tools are trained on pharmaceutical chemistry and fail in this domain, we built a model grounded in the judgment of four senior industrial explosives chemists. To our knowledge the first of its kind for energetic materials, it predicts synthetic difficulty with an accuracy that rivals the agreement among the experts themselves.

Together, these advances establish a design pipeline that yields molecules which are both high-performing and realistically makeable. As a demonstration, five computer-designed candidates, validated with high-level quantum chemistry and empirical correlations, outperformed RDX, a widely used benchmark military explosive, on every detonation metric, with the best exceeding even the more powerful HMX. This work highlights how domain-aware generative design can accelerate the discovery of next-generation energetic materials while keeping synthesis firmly in view.