AI Can Generate Novel High-Energy Sustainable Aviation Fuel Molecules

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Full Methods&Data:

UCL

1. Why Do Planes Need Better Fuel?

Aviation = 2.5% global CO_2 [1] and demand is rising

Current sustainable aviation fuels (**SAFs**) are **costly** with **inferior properties**. Traditional fuel discovery is slow & expensive.

Generative AI is widely used in drug discovery, but only limited use for aviation fuel.

Aim: Use Generative AI to design novel, high-energy, and sustainable fuel molecules.

2. How Can AI Design Molecules?

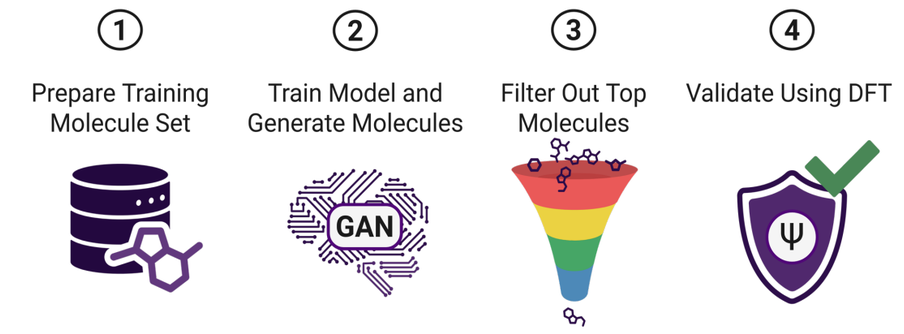


Fig. 1. Four-step methodology. **DFT**: density functional theory.

Here, Generator and Discriminator consist of transformer encoders. The model also includes other heuristics to improve **stability** and **diversity**.

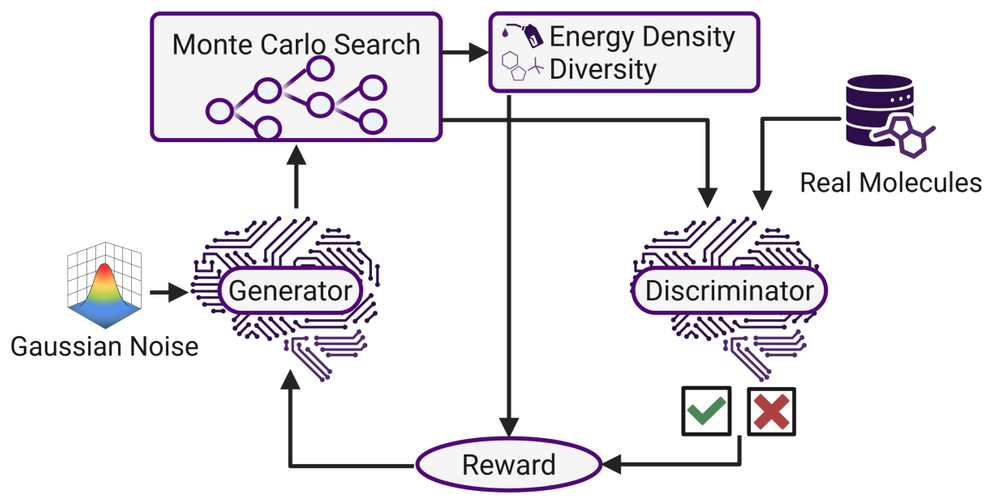


Fig. 2. Schematic of the used Generative Adversarial Network (**GAN**). Model is based on TenGAN [2].

3. What Did We Discover?

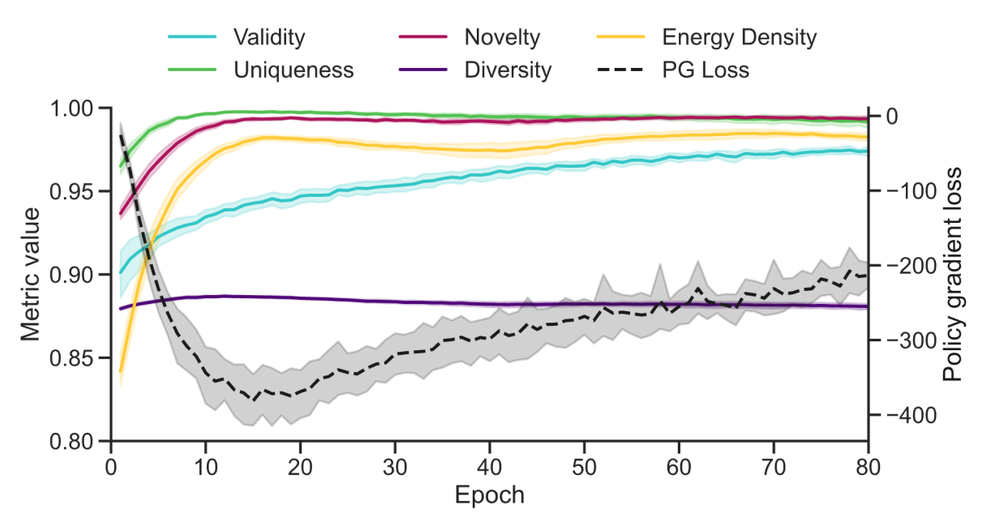


Fig. 3. Model metrics improve steadily during training (99 % CI shown).

AI learns to make better molecules: the model improved, producing highly valid, unique, and novel molecules with high predicted energy density.

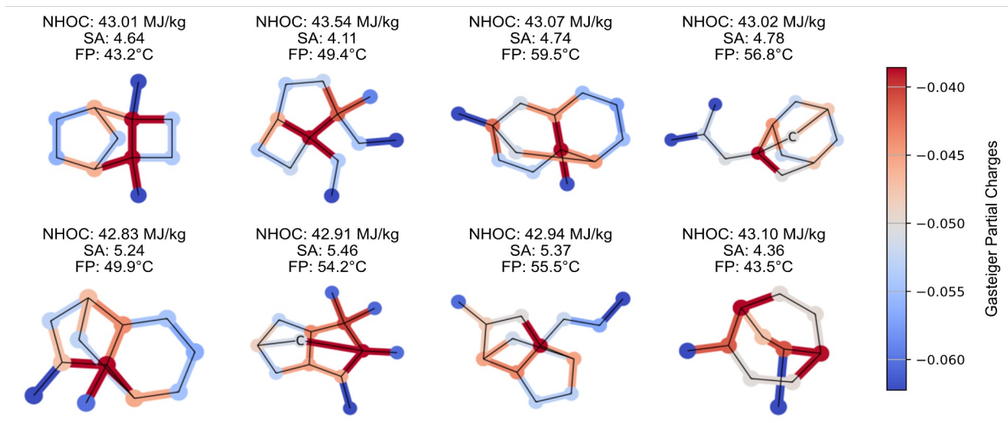


Fig. 4. Top candidate molecules after screening process. **NHOC**: net heat of combustion, **SA**: synthetic accessibility, **FP**: flash point.

Systematic property filtering works: 10 000 generated molecules were filtered to top 250.

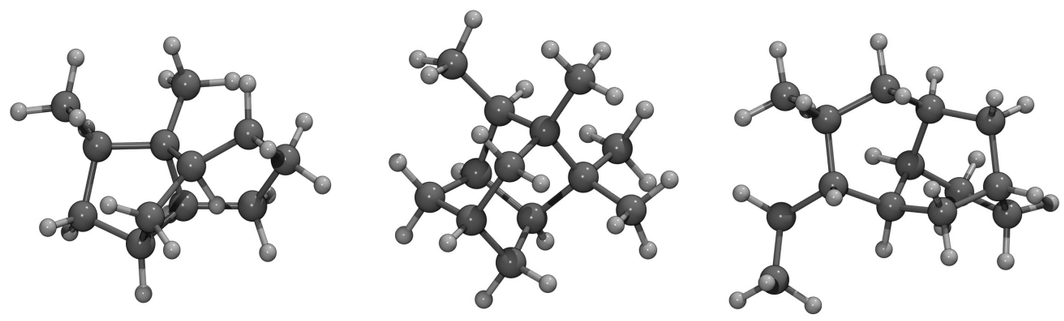
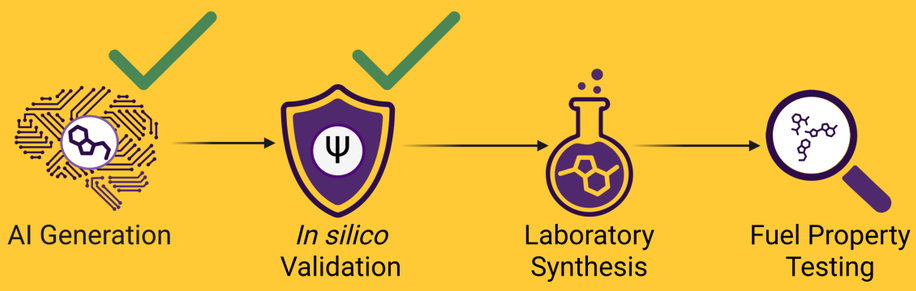


Fig. 5. 3D optimised structures of selected molecules.

Final candidates rival best aviation fuels: fuels in Fig. 5 exceed Jet-A in NHOC and pass the ASTM D7566 [3] requirements for all predicted properties.

4. What is Next?

- Our **generation-screening workflow** can produce **high-quality SAF candidates**.
- **Next steps:** synthesis pathway analysis, synthesis of molecules and property testing.



References

[1] Ritchie H. What share of global CO_2 emissions come from aviation? Our World in Data. 2024 Apr 8 [cited 2025 Jul 23]. Available from: https://ourworldindata.org/global-aviation-emissions.
[2] Li C, Yamanishi Y. TenGAN: Pure transformer encoders make an efficient discrete GAN for de novo molecular generation. In: Dasgupta S, Mandt S, Li Y, editors. Proceedings of the 27th International Conference on Artificial Intelligence and Statistics; 2024 May 2-4; Valencia, Spain. Proceedings of Machine Learning Research. 2024;238:361-369. Available from: https://proceedings.mlr.press/v238/li24d.html
[3] ASTM International. ASTM D7566-24d: Standard Specification for Aviation Turbine Fuel Containing Synthesized Hydrocarbons. West Conshohocken (PA): ASTM International; 2024.