

CuspAI: AI-Driven Material Science

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Abstract

Climate change represents one of humanity's most urgent challenges, with 2024 breaking the 1.5°C global warming barrier amid mounting evidence of accelerating environmental impacts. Addressing this crisis requires revolutionary approaches to materials science that can drastically reduce greenhouse gas emissions. CuspAI is a frontier AI company on a mission to build the breakthrough materials needed to power human progress. By harnessing the transformative potential of artificial intelligence, we are fundamentally reimagining the materials discovery process.

Our material science platform is powered by machine learning, and is capable of computational design and discovery for a wide range of applications. Our initial focus is on developing next-generation materials capable of making frontiers like carbon capture affordable and scalable.

Traditional materials development approaches face significant limitations:

- Computational approaches typically lack adequate robustness for reliable application
- Conventional material development typically requires 15 - 25 years [1] from concept to scalable material
- Conventional screening methods evaluate only dozens of candidates annually

These constraints have significant implications for carbon capture, as carbon capture costs are prohibitive and largely a function of the performance of the underlying materials. We address this challenge by assembling a top team of material scientists, physics, chemists, chemical engineers, and machine learning practitioners.

In this poster, we outline CuspAI's mission and outline our platform; an accelerated materials discovery pipeline that links generative AI models with virtual twin assessment capabilities. This integrated system enables rapid feedback loops between material structure, computational chemistry tools, and application-based performance predictions, dramatically shortening development timelines.

Beyond carbon capture, our platform is designed to extend into other frontiers including semiconductors and water purification, putting CuspAI at the forefront of AI-driven materials science.

References

[1] Correa-Baena, Juan-Pablo, et al. "Accelerating materials development via automation, machine learning, and high-performance computing." *Joule* 2.8 (2018): 1410-1420.