

The future of materials science with AI: Max Welling and Cusp AI

The AI revolution is not only making strides in robotics, but also has the potential to transform materials science. Max Welling, a researcher and founder of Cusp AI, is working on a platform for developing new materials using AI.



Prof. Dr. Max Welling, founder of Cusp AI

CuspAI, a company with about 20 employees, is focusing on AI-based materials research.

The company is developing a platform that serves as a kind of 'search engine for materials'. This uses machine learning to design new materials for various applications. The first areas of application include:

- **gas separation and carbon capture:** new materials could significantly improve the efficiency of CO₂ separation.
- **Semiconductor materials:** As the miniaturisation of chips continues, materials research is becoming increasingly important to find new, more powerful alternatives to silicon.

The platform is based on generative AI models that create and simulate new molecules. In addition, CuspAI uses physics-based models to predict the properties of these molecules.

Technological foundations and AI models

The platform relies on various methods:

- **generative models** that design new molecules and condition their properties.
- **force fields** that enable physical simulations by calculating the energies and forces of atoms.
- **property predictors** that bypass simulations

by directly predicting material properties.

- **AI-powered search agents** that efficiently filter the best materials from a large set of potential combinations.

Welling emphasises that AI is enabling tremendous progress in materials research. Simulations that used to take weeks can be done in seconds with AI-powered models.

Data sources and collaboration with companies

CuspAI draws on various data sources, including:

- Public databases such as Materials Project and Nomad.
- Company-specific data provided through collaborations with companies.
- In-house simulations that generate synthetic data to improve the AI models.

A particular challenge is combining domain-specific knowledge with AI. Welling describes how many companies have data but not the necessary machine learning experts to use it efficiently. CuspAI offers a bridge between materials science and AI.

For the next phase, Welling is looking for excellent researchers in the field of machine learning and chemistry. The company's locations – including Cambridge, Amsterdam and Berlin – offer an attractive environment for European talent.