

REFORMULATE PLASTICS FOR SAFETY AND SUSTAINABILITY



Replacing toxic ingredients while also retaining technical performance

The Research Group

- **NSF funded project**
- MIT, Cornell and Swansea Universities with Citrine Informatics

The Problem

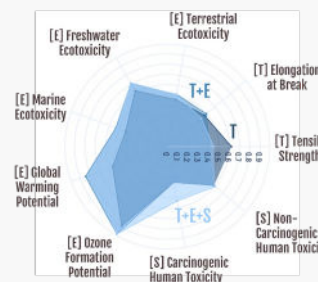
- Toxic additives in PVC plastics are becoming increasingly scrutinized and banned, particularly **phthalate plasticizers**
- However, non-toxic replacements have unknown impacts on PVC mechanical performance
- Identify PVC formulations that remove phthalates but retain plasticity

The Process

- Gathered data on plastic ingredients (including plasticizers, fillers, stabilizers, lubricants) and PVC formulations
- Built ML models to predict mechanical **performance and toxicity**
- **Optimized plastic formulations** for mechanical performance with and without toxicity constraints

The Outcome

- **Quantitative trade-off** of technical (T) performance, with and without ecological (E) and societal (S) constraints
- Engineers can **determine cost** of satisfying regulations or supply-chain constraints



Normalized properties, higher is better (e.g., less toxic)



Saal, Hegde, Ortiz, Spero, et al. , publication in preparation