INTRODUCE

Royal Society URF at University of Cambridge
CSO at startup Intellegens commercializing the work
Develop machine learning to learn from sparse and noisy experimental data
License software product to design drugs, chemicals, and materials

WHAT DOES MODELLING AND AI DESIGN MEAN FOR YOU

MODEL:
take input parameters - what can tune in the factory to
predict result of experiments that measure performance, but cheaper and quicker

AI DESIGN
Model is artificial intelligence, given a set of target properties
it finds the design parameters that fulfil them or reports not possible

HOW TO GET STARTED USING NEW MODELING AND DESIGN TECHNIQUES

Create simplified dataset with only essential columns eg $y=x$
Plot it to gain physical intuition of trends
Apply simplest open source model
Plot predictions to verify that it has understood trends
Progressively build complexity to include more information
Ensure doing proper blind validation of the model, probably through cross-validation

WHAT ROLE DOES OPEN SOURCE SOFTWARE HAVE

AI requires a lot of data so sharing increases pool
Research funded open data helps, consortiums also possible eg OPTIMADE
Also common ontologies so easier to share data (EMMO) European Materials & Modeling Ontology
Open source helpful in research Universities when trying new ideas so
can readily access standard method, use in a terminal, and modify it

HOW DOES MANUFACTURING INFORM YOUR MODELS AND DESIGNS

20% value of material in first working prototype, 80% value in factory so
crucial to do manufacturing correctly
Obscure variables such as which window open can only be captured
with AI, not amenable to first principles
Often composition is certified so want to leave fixed, but manufacturing
parameters can be varied to improve properties without recertification