



EMPOWERING SCIENTISTS THROUGH DATA & AI

FLORENCIA
PAREDES
SR PRODUCT MANAGER

CITRINE[®]
INFORMATICS



CITRINE
INFORMATICS,
LEADER IN
MATERIALS
INFORMATICS

WE BUILT THE
WORLD'S FIRST
MATERIALS AND
CHEMICALS FOCUSED
AI PLATFORM



THE ROLE FOR ML IN MATERIALS SCIENCE?

SHOULD WE ABANDON KNOWN THEORY AND DOMAIN KNOWLEDGE,
AND TRY TO OUTSOURCE SCIENTIFIC THINKING TO AI?

ABSOLUTELY NOT!

AI IS POWERFUL COPILOT,
BUT WE STILL NEED
EXPERTS

*“What would’ve taken **years**, Citrine narrowed it down **to days**.”*

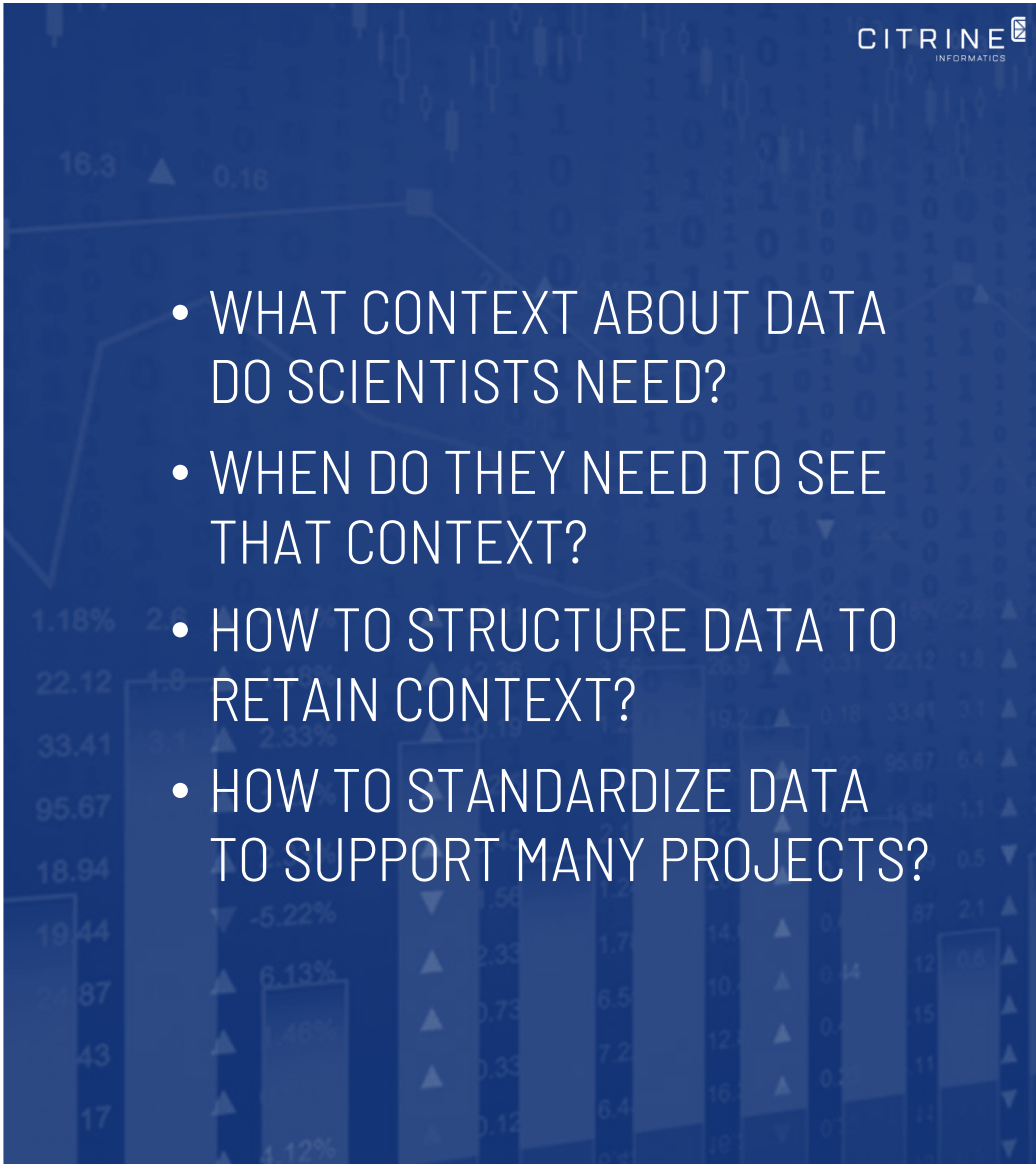
- Dr. Hunter Martin, HRL Laboratories

DOMAIN KNOWLEDGE
IS KEY TO LEVERAGE DATA AND ML
FOR ACCELERATING MATERIALS
DEVELOPMENT

1. MATERIALS DATA IS **MESSY**
2. MATERIALS DATA IS **SCARCE**
3. TEAMS LACK **COLLABORATION**

MATERIALS DATA IS MESSY

1. DEPENDENT ON CONTEXT
2. DISCONNECTED
3. MANY FORMATS

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- WHAT CONTEXT ABOUT DATA DO SCIENTISTS NEED?
 - WHEN DO THEY NEED TO SEE THAT CONTEXT?
 - HOW TO STRUCTURE DATA TO RETAIN CONTEXT?
 - HOW TO STANDARDIZE DATA TO SUPPORT MANY PROJECTS?

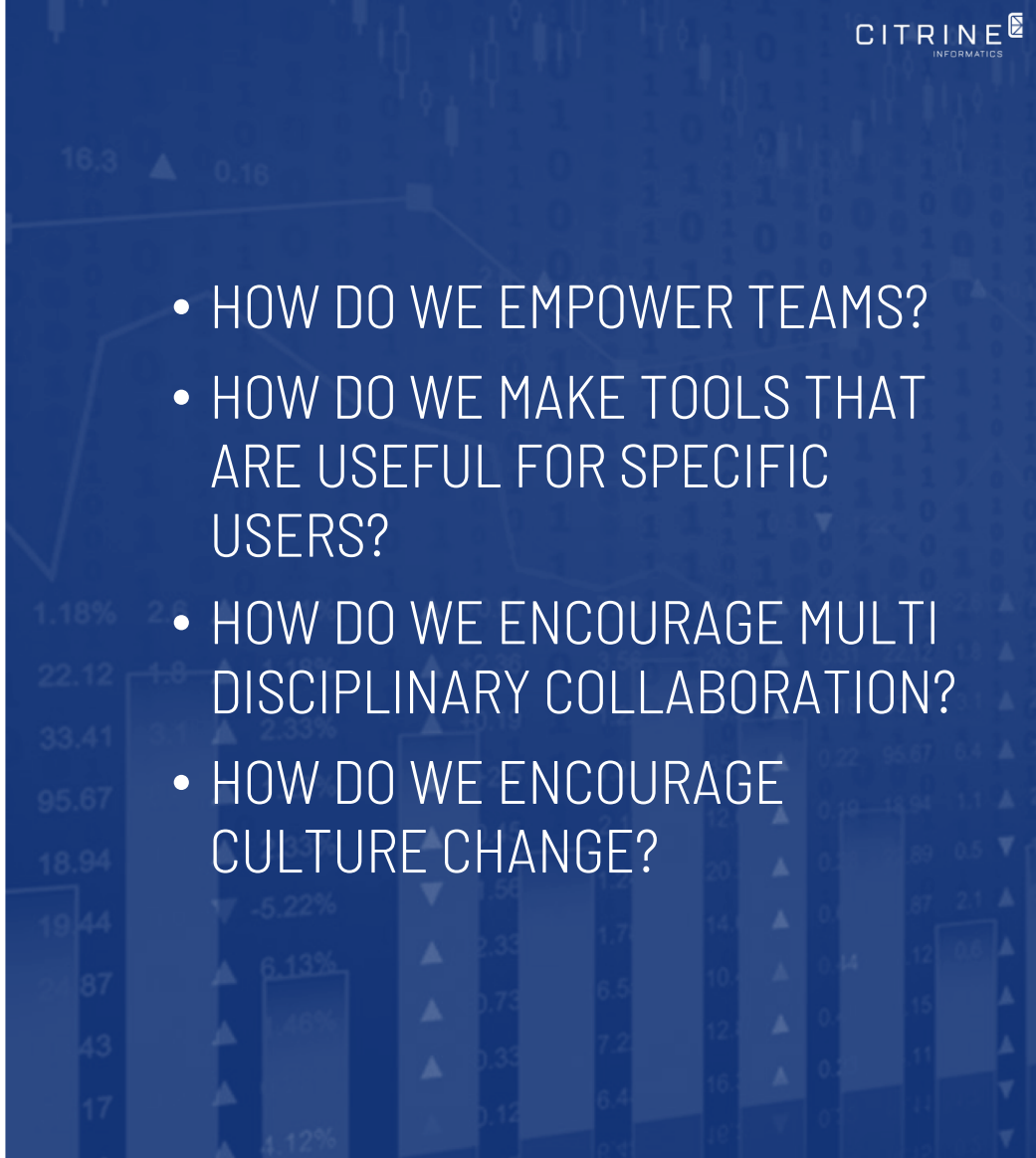
MATERIALS DATA IS SCARCE

1. SMALL DATASETS
2. SPARSE DATA
3. REQUIRES EXTRAPOLATION

- HOW DO SCIENTISTS LEVERAGE MORE VALUE FROM THEIR DATA?
- HOW DO SCIENTISTS DEFINE THEIR NEXT EXPERIMENT TODAY?
- WHAT DO THEY NEED TO TRUST A MODEL?

TEAMS LACK COLLABORATION

1. TOOLS FOR USERS
2. SCALE FOR MANY
3. CULTURE CHANGE

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- HOW DO WE EMPOWER TEAMS?
 - HOW DO WE MAKE TOOLS THAT ARE USEFUL FOR SPECIFIC USERS?
 - HOW DO WE ENCOURAGE MULTI DISCIPLINARY COLLABORATION?
 - HOW DO WE ENCOURAGE CULTURE CHANGE?

AI@SCALE

MATERIALS
SCIENTISTS

DATA SCIENTIST



EMPOWERING TEAMS TO SOLVE PROBLEMS WITH DATA AND AI

THANK YOU!

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