


AI + Materials Discovery: A Hybrid Approach



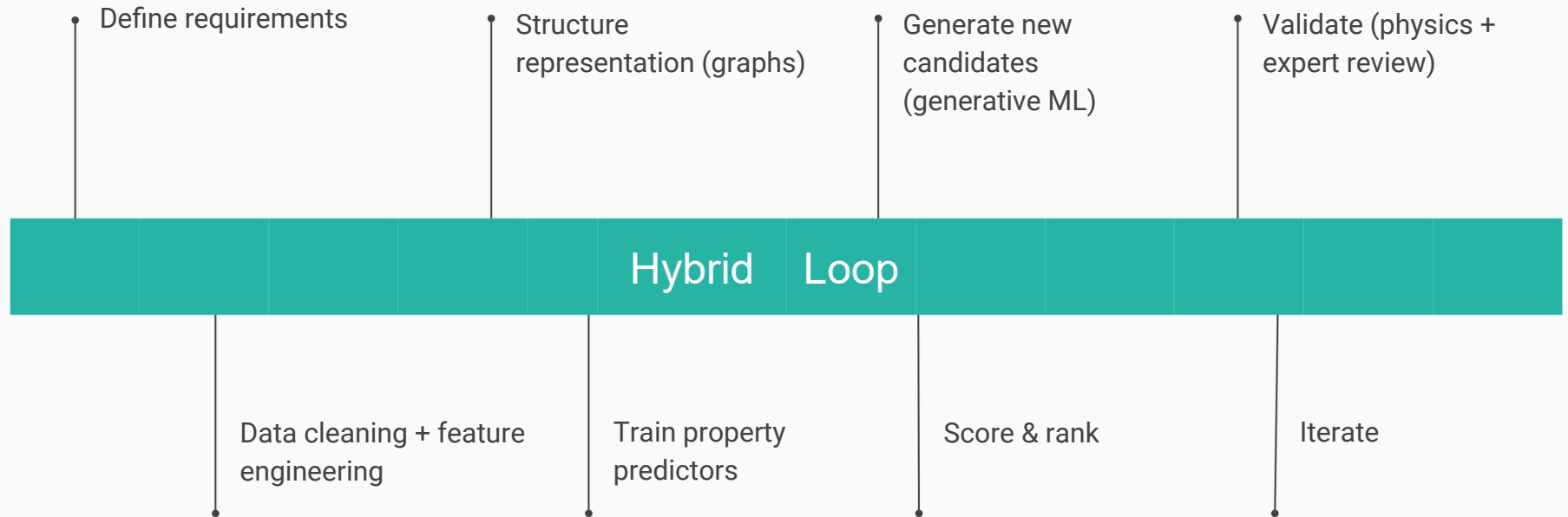
**THE REMOTE
CONSULTANT**
with Sebastian



How do we go beyond known datasets?

Step-by-Step Approach

From Data to Discovery



Suitable ML Models

GNNs

Understand
structure-property
relations

Learn directly from
atomic structures



Generative Models

Propose new
candidates

Create **new formulas &
structures**



Reinforcement Learning

Optimize for specific
needs

Steer discovery
towards requirements





Value & Differentiation

Why This Approach Works

