

# Rebooting Materials Design and Discovery

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6<sup>th</sup> European Conference on Computational Mechanics (ECCM 6)

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# Example for Follow-on Session

# Materials Design Translation Recommendations

- Choosing most suitable modeling approach and executor:
  - Funnel approach generally useful
    - Lowest computational cost method on widest range of materials
    - Most expensive computational cost method on smallest pre-screen range of materials
  - Translators must be flexible and willing to ask for help
    - Figures-of-merit and parameters for higher-level models are viable
- General criteria used:
  1. Material property targets
  2. Feasible material composition(s)
  3. Processing conditions
  4. Potential unintended materials
  - Customer request usually includes #1 (sometimes #2), but translators need to tease out remaining in discussions and literature research
- Major bottlenecks/challenges of a translator:
  - Modeling iterations to get a reliable property methodology workflow
  - Computational time
  - Search for composition that meets the property requirements