

# Automating Transferable Coarse-Model Generation and Back-Mapping with an Open Source Toolchain

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## Aims

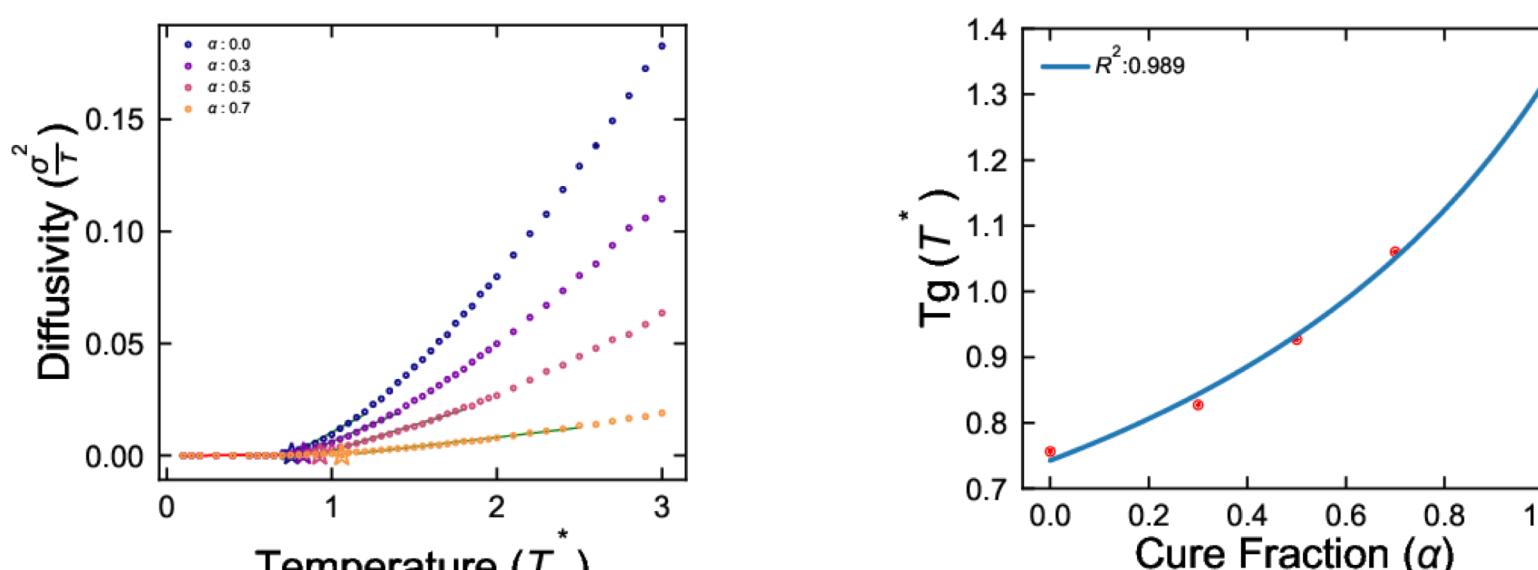
- Experimentally relevant structure predictions enabled with coarse-grained models
- Transferable, Reproducible, Usable, Extensible simulations

## Approach: Improve access

- Software interfaces
  - SMILES strings
  - mBuild+foyer+freud+signac = MSIBI
- Community interfaces
  - Inclusive dev meetings
  - Code of conduct
  - Best practices

## Results

- Experimentally relevant time and length scales
- Charge transport calculations for organic photovoltaics:  
 $N = 3.8e5$ ,  $L = 15 \text{ nm}$ ,  $t = 3 \mu\text{s}$
- Reacting epoxy thermoset structure, Tg predictions:  
 $N = 4e6$ ,  $L = 0.1 \mu\text{m}$ ,  $\alpha \leq 98\%$



# Starting simply and being nice maximizes large-scale simulation impact



Get the code, paper, and more!

