Many interesting phenomena cannot be studied at a single spatiotemporal scale and instead require information over a spectrum of length and timescales to provide a good description. Effective coarse-graining schemes that traverse electronic to mesoscopic length and timescales are critical to the success of these efforts. Here, we describe recent developments in the group that address critical problems related to coarse-grained simulations.

### Electronic Coarse-graining

In semiconducting soft materials, accurately characterizing configuration-dependent electronic structure is critical to predictive modeling. Coarse-graining is a powerful avenue for accessing the relaxation times of soft materials, but the approach requires expensive atomistic backmapping and quantum chemistry to determine the optoelectronic behavior.

Existing means of determining electronic structure from coarse-grained degrees of freedom require hand-picked degrees of freedom and cleverly chosen model hamiltonians:

\[
H = \sum \left( \frac{1}{2} c_i^\dagger c_i^\dagger c_i c_i - t_{ij} c_i^\dagger c_j + c_j^\dagger c_i \right)
\]

**Dihedral-based tight-binding Hamiltonian**

Advanced machine learning algorithms present the possibility for regressing an optimal "Hamiltonian" directly to CG degrees of freedom, without human bias towards the physical Hamiltonian. This has the potential to improve the accuracy, speed, and ease of soft material modeling.

### ANN - Electronic Coarse-graining

We have developed an artificial neural network electronic coarse-graining (ANN-ECG) approach to efficiently map configuration-dependent atomistic electronic structure to coarse-grained configurational degrees of freedom. ANN are utilized to directly regress configuration dependent electronic structure to CG degrees of freedom.

- No atomistic backmapping.
- Improved accuracy over physics-based models.
- Identification of optimal CG representations.
- Accelerates morphology exploration by ~10^3.

**ANN-ECG Outperforms Existing Physics-Based Models**

**Future Directions**

- Combine GBCG and ANN-ECG to search for optimal CG representations for a given soft semiconducting material.
- Leverage GBCG in adaptive resolution simulations to exploit the hierarchical nature of the generate models.

### References