Outline

**Introduction/Goal**

Current molecular dynamics simulations are not good at modeling reactive systems efficiently – classical force fields fail, reactive are intensive and highly specific, quantum mechanical models are limited to short length and timescales (Univ Frame). GMP utilizes physically relevant multi-pole expansions of electron density around atoms to yield feature vectors that interpolate between element types and have a fixed dimension regardless of the number of elements present – good for scaling?

Missing universally applicable descriptors (feature vectors) Most common problem is scaling of feature vectors with number of elements. GMP utilize implicit description of electron density – feature vector dimsnsion is independent of number of elements. Electron density as input makes them suitable for universal ML models – straightforward to extend to charged atoms or magnetic moments. Allows more efficient SNN. Related to multi-pole expansion of electron density making them physically relevant and systematically improvable.

Interesting/useful to explore application of GMP expansion to charged, magnetic moment, all-electron density, spin density, self-consistent electron density?

Modifying valence density representation, optimizing feature selection, systematic optimization of SNN architecture

Would multi-pole include more non local information?

Testing for reactive systems – combining with MD simulations, modeling breakdown of polymeric systems?

**Strategy**

Translate the mathematical framework to account for polymeric systems – seems like it could be minimal work – inherently challenging – challenge GMP?

Incorporate into Sparc Simulation package

Perform screening – collaborate with experimentalist. Could use this as a metric

**Impact**

Plastics pollution is a serious problem – need solutions that don’t exist. Effective screening tools necessary. Predicated on idea of programmed decomposition.

**Keywords**

Feature vectors; translational, rotational (norm), permutation invariances; feature vectors; Gaussian basis functions;

**Hypothesis**

GMP can be used to fingerprint polymeric systems which will enhance the level of detail of these simulations and enable the modeling of reactive environments.

Secondary – blend of different simulation types – course grained/atomistic

**References**

Polymers designed to degrade upon external stimulus