



ethane geometries using feature set B, and Figure 3a presents data. The ML model is first trained on 100 methane and 300 and isobutane CC2D energies from shorter alkane training family of covalently bonded molecules by predicting butane

As a second example, we examine transferability within a

Figure 4 explores ML predictions for methanol using a training

C. Transferability across Molecules and Elements

that appear in the test data.

training data increasingly represent chemical environments training data, and demonstrates systematic improvability as the even for molecules with atom-types that are not included in the encompassing transferability, provides good prediction accuracy these results directly illustrate that the ML model exhibits examples are still not included in the training data. Regardless, while improved, remain slightly larger since tertiary carbon of the butane ML predictions, whereas the isobutane errors, information about secondary carbons to the particular parent data. In Figure 3b, the propane training data provides which include atom-types that are not included in the training model predicts the energies for butane and isobutane, both of not tertiary carbon atoms; it is thus notable how well the ML 3a, the training data includes examples of neither secondary whereas isobutane includes a tertiary carbon atom. In Figure molecule includes only primary and secondary carbons, are included in the training data. The unbranched butane