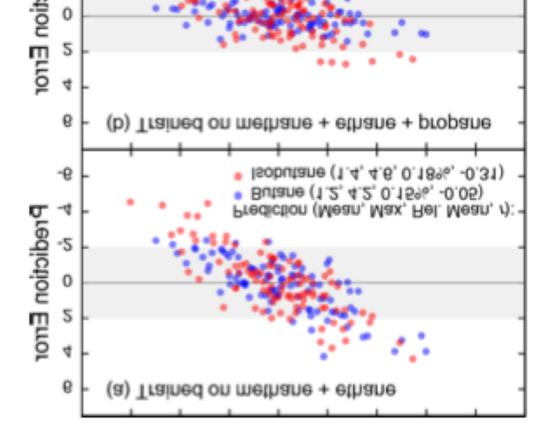
Journal of Chemical Theory and Computation

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



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 encouraging 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 benefit 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 nor 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

C. Transferability across Molecules and Elements. Figure 4 explores ML predictions for methanol using a training