A Molecular Model for Chiral Symmetry Breaking FOLARIN LATINWO, FRANK STILLINGER, PABLO DEBENEDETTI, Princeton University — In this work, we present a new class of molecular models for chiral phenomena in condensed matter systems. A key feature of these models is the ability of the four-site (tetramer) “molecules” to inter-convert between two distinct chiral forms (enantiomers). Given this feature, we use analytical theory and computer simulations to investigate the emergent chiral properties (including symmetry breaking) over a range of conditions. In particular, we consider the single-molecule level and condensed-phase behavior of our model system. Interestingly, we find that our liquid-phase predictions are in excellent agreement with recent experimental reports on chiral self-sorting in isotropic liquids. From this perspective, our model demonstrates accurate predictive capabilities, as well as a platform for understanding the microscopic origins of a variety of chiral phenomena. In a broader context, we anticipate that this class of models will be relevant to chirality-dominated areas such as the pharmaceutical industry and pre-biotic geochemistry.

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