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Persistent medium-range order and anomalous liquid properties of $Al_{1-x}Cu_x$ alloys[1] JOONGOO KANG, JUNYI ZHU, SU-HUAI WEI, National Renewable Energy Laboratory, Golden, CO, USA, ERIC SCHWEGLER, Lawrence Livermore National Laboratory, Livermore, CA, USA, YONG-HYUN KIM, KAIST, Daejeon, Korea — The development of short-to-medium-range order in atomic arrangements–that is, the aggregation or packing of short-range order (SRO) atomic clusters–has generally been observed in noncrystalline solid systems such as metallic glasses. Whether such medium-range order (MRO) can exist in materials at well above their melting or glass-transition temperature, manifesting itself in some observable property such as a liquid–liquid transition, has been a long-standing important scientific challenge. Here, using *ab initio* molecular dynamics simulations, we show that a novel, persistent MRO exists in liquid Al-Cu alloys, both in the nano- and bulk phases, near the composition of $CuAl_3$. In a sense, the MRO liquid lies in between glasses and normal liquids, and thus it exhibits anomalous liquid properties. Our *ab initio* calculations provide a detailed atomistic description of the MRO as well as a microscopic explanation for its formation via a percolation-like transition. Interestingly, we find that the appearance of MRO in the liquid phase manifests itself in a substantially enhanced viscosity that is consistent with a previously unexplained experimental observation of a peak in the viscosity of Al-Cu alloys.

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