Abstract Submitted
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Morphology of hydrocarbon films on decagonal Al-Ni-Co quasicrystalline surfaces[1] WAHYU SETYAWAN, Duke University, Department of Mechanical Engineering and Materials Science, RENEE D. DIEHL, Penn State University, Department of Physics, MAJID KARIMI, Indiana Univeristy of PA, STEFANO CURTAROLO, Duke University, Department of Mechanical Engineering and Materials Science and Department of Physics — Lubricants can affect quasicrystalline coatings by modifying commensurability. We present simulation studies of physically adsorbed hydrocarbons on a decagonal surface of a Al-Ni-Co quasicrystal. We use the Grand Canonical Monte Carlo technique with novel embedded-atom-method potentials fitted to *ab initio* calculations and standard hydrocarbons interactions. Methane forms pentagonal structure, benzene monolayer adsorbs in hexagonal domains with 5 orientational degeneracies induced by the substrate, propane forms pentagonal domains with significant disorder, hexane and octane monolayers shows linear ordering. The results support the potential use of quasicrystals as low friction coatings.

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