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Origin and structure of polar domains in doped molecular crystals IDO AZURI, ELENA MEIRZADEH, Weizmann Institute of Science, YUBO QI, University of Pennsylvania, DAVID EHRE, Weizmann Institute of Science, ANDREW RAPPE , University of Pennsylvania, MEIR LAHAV, LEEOR KRONIK, IGOR LUBOMIRSKY, Weizmann Institute of Science — Doping is a primary tool for the modification of the properties of materials. Occlusion of guest molecules in crystals generally reduces their symmetry by the creation of polar domains, which engender polarization and pyroelectricity in the doped crystals. Here we describe a molecular-level determination of the structure of such polar domains, as created by low dopant concentrations (<0.5%). The approach comprises crystal engineering and pyroelectric measurements, together with dispersion-corrected density functional theory and classical molecular dynamics calculations of the doped crystals, using neutron diffraction data of the host at different temperatures. This approach is illustrated using centrosymmetric α-glycine crystals doped with minute amounts of different L-amino acids. The experimentally determined pyroelectric coefficients are explained by the structure and polarization calculations, thus providing strong support for the local and global understanding of how different dopants influence the properties of molecular crystals.

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