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Probing the molecular structure of doped sites within crystals by Pyroelectricity and Dispersion Corrected DFT modeling ELENA MEIRZADEH, IDO AZURI, DAVID EHRE, Weizmann Institute of Science, ANDREW M. RAPPE, University of Pennsylvania, MEIR LAHAV, LEEOR KRONIK, IGOR LUBOMIRSKY, Weizmann Institute of Science — We describe the analysis of polar architectures at the nanoscale by pyroelectric measurements and DFT. Controlled doping of crystals is a primary tool for modification of the properties of materials. Doping of non-polar molecular crystals with "tailor-made" auxiliaries often reduces their symmetry, and converts them into polar mixed crystals. Such crystals are pyroelectric, *i.e.* they display temporary surface charge if subjected to a temperature change. When the non-polar crystals of the amino-acids are doped with different amino acids of concentrations as low as <0.2%, they display measurable pyroelectric effect. Since such minute amount of guest creates measurable macroscopic polarization, implies a local polar dislocation of the neighboring host molecules. We demonstrate here, that the value and the temperature dependence of the pyroelectric coefficient, provides intimate information on the molecular packing arrangement of the doped sites. Different amino acids as dopants induce different pyroelectric effects: The pyroelectric coefficient is a) not temperature dependent; b) changes its sign upon heating. These differences were explained by the determination of the polar domains at the molecular level by the DFT.

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