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Effect of polar surfaces on organic molecular crystals[1] ONISE SHARIA, ROMAN TSYSHEVSKIY, MAIJA KUKLJA, University Of Maryland College Park, UNIVERSITY OF MARYLAND COLLEGE PARK TEAM — Polar oxide materials reveal intriguing opportunities in the field of electronics, superconductivity and nanotechnology. While behavior of polar surfaces has been widely studied on oxide materials and oxide-oxide interfaces, manifestations and properties of polar surfaces in molecular crystals are still poorly understood. Here we discover that the polar catastrophe phenomenon, known on oxides, also takes place in molecular materials as illustrated with an example of cyclotetramethylene tetranitramine (HMX) crystals. We show that the surface charge separation is a feasible compensation mechanism to counterbalance the macroscopic dipole moment and remove the electrostatic instability. We discuss the role of surface charge on degradation of polar surfaces, electrical conductivity, optical band-gap closure and surface metallization.

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