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Spontaneous polarization and piezoelectricity in polar molecular crystals IVO BORRIELLO, University of Naples Federico II, Naples Italy, GIOVANNI CANTELE, CNR-COHERENTIA, University of Naples Federico II, Naples Italy, DOMENICO NINNO, GIUSEPPE IADONISI, University of Naples Federico II, Naples Italy — Molecular materials with a polar arrangement of the constituent dipoles are good candidates for exhibiting piezoelectric properties, directly related to the strain-induced polarization. The metal-organic molecular crystal (4-dimethylaminopyridyl)bis(acetylacetato)zinc(II) (ZNDA) has been investigated from first principles. The spontaneous polarization and the piezoelectric properties have been studied by means of the modern theory of polarization, focusing on the relation between the piezoelectric properties of the organic crystal and the electronic properties of the polar molecule.

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