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Abstract:	Combining density-functional theory and many-body approaches we investigate the origin of the ferroelectric phase generally observed in TMTTF2-X organic crystals. We solve by means of mean-field theory and exact diagonalization a two-dimensional tight-biding model built from density-functional theory calculations and we show that short-range interactions stabilize a dimerized charge-ordered state in a wide range of parameters. Two different charge-ordering patterns are found; these correspond to those observed for X=PF6 and X=SCN. In the former case, a lattice dimerization couples with the charge ordering, leading to a polarization. Due to the interplay between charge and magnetic ordering, such polarization appears to be magnetically driven, thus revealing TMTTF2-PF6 as a multiferroic material.
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