Abstract Submitted
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Molecular Crystals, a test system for weak bonding.[1] BERNARD DELLEY, Paul Scherrer Institut Switzerland, TEODORA TODOROVA, Paul Scherrer Institut Switzerland — Intermolecular binding in molecular crystals are due to electrostatic and Van-der-Waals interactions. Crystal parameters are crucially dependent on the accuracy of the electronic model. We investigate sets of molecular crystals, classified by the lowest non-vanishing molecular multipole moment, with density functional theory. We find that certain density functional approximations give an almost surprisingly good description of such lattices, deteriorating only moderately going from molecules with dipole moment, to ones with quadrupole and to even higher symmetry molecules, where finally Van- der-Waals interactions dominate at large distance. For the best performing density functional approximations, even the VdW subset has an error range of calculated lattice parameters comparable to crystals with covalent, ionic or metallic bonds.

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