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Effect of packing motifs on the energy ranking and electronic properties of putative crystal structures of tricyano-1,4-dithiino[c]-isothiazole FARREN CURTIS, XIAOPENG WANG, NOA MAROM, Carnegie Mellon University — We present an analysis of putative structures of tricyano-1,4-dithiino[c]- isothiazole (TCS3), generated within the sixth crystal structure prediction blind test. Typical packing motifs are identified and characterized in terms of distinct patterns of close contacts and regions of electrostatic and dispersion interactions. We find that different dispersion-inclusive density functional theory (DFT) methods systematically favor specific packing motifs, which may affect the outcome of crystal structure prediction efforts. The effect of crystal packing on the electronic and optical properties of TCS3 is investigated using many-body perturbation theory within the GW approximation and the Bethe–Salpeter equation (BSE). We find that a structure with $Pna2_1$ symmetry and a bilayer packing motif exhibits intermolecular bonding patterns reminiscent of pi–pi stacking and has markedly different electronic and optical properties than the experimentally observed $P2_1/n$ structure with a cyclic dimer motif, including a narrower band gap, enhanced band dispersion, and broader optical absorption. The $Pna2_1$ bilayer structure is close in energy to the observed structure and may be feasible to grow.

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