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Magnetism and superconductivity in modulated FeTe systems. KALUM PALANDAGE, Trinity College, Hartford, CT, GAYANATH FERNANDO, University of Connecticut, Storrs, CT, ARMEN KOCHARIAN, California State University, Los Angeles, CA — We examined the interplay between magnetism and superconductivity by monitoring the non-superconducting chalcogenide FeTe. We studied its transitions under insertion of oxygen, iron and vacancies of iron using spin-polarized band structure methods (LSDA with GGA) starting from the collinear and bicollinear magnetic arrangements. A supercell with 8-Fe and 8-Te atoms was used so that it can capture local changes in magnetic moments. The calculated values of magnetic moments agree well with available experimental data while some of the modulations lead to significant changes in the bicollinear or collinear magnetic moments/arrangements. The total energies of these systems indicate that the collinear-derived structure is more favorable prior to a possible superconducting transition.

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