

Supplemental Materials: Magnetic Stability, Fermi Surface Topology, and Spin-Correlated Dielectric Response in Monolayer 1T-CrTe₂

A. Energy Convergence With Respect To Sampling In The Unit Cell of Ferromagnetic CrTe₂

Relaxation is performed on a unit cell until the force on each atom becomes less than 0.002 eV/Å and the total energy converges to within 10⁻⁸ eV. A cutoff energy surface of 600 eV was used for the plane-wave-basis. A Γ -centered Monkhorst-Pack of $13 \times 13 \times 1$ was used to sample the Brillouin zone for relaxation. After relaxation, the mesh was changed to be $n \times n \times 1$ where: $3 \leq n \leq 15$. Colinear self-consistent calculations were performed using different n values to find a suitable mesh for the unit cell.

In the figure below, the ground energy of the unit cell with respect to the size of a mesh $n \times n \times 1$ is shown. The value of n was allowed to go up to 25. Notice how the energy oscillates around the value $E = -16.2625$ eV, especially for values where $n \geq 10$. This oscillatory behavior is another indicator that the chosen mesh is suitable for the calculation. The mesh sizes of the supercells were picked with this criterion in mind.

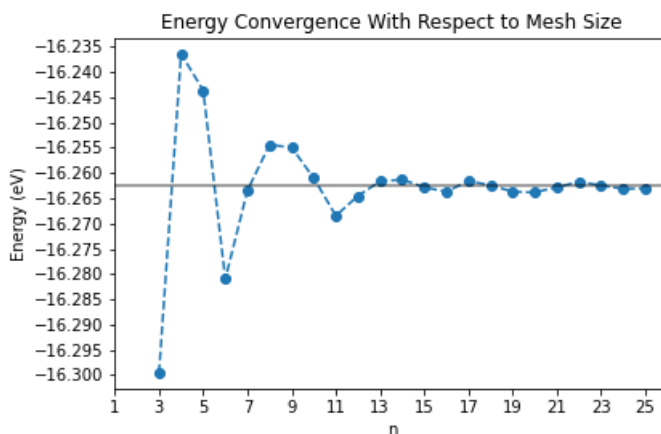


FIG. S1: Energy Convergence as a function of sampling points.

B. Ground Energy Convergence With Respect to Cutoff Energy In The Unit Cell of Ferromagnetic CrTe₂

The relaxed structure generated in the previous section was also used to perform colinear self-consistent calculations to test the convergence of the ground state energy against the energy cutoff surface used for the plane-wave-basis set. A mesh of $13 \times 13 \times 1$ was used for the calculation. The self-consistent calculations were performed until the total energy difference reached 10⁻⁸ eV.

$E_{cutoff}(eV)$	$E_{total}(eV)$
400	-16.260964
450	-16.261668
500	-16.262638
550	-16.262849
600	-16.262793
650	-16.262816
700	-16.263001

TABLE S1: Ground Energy Convergence with respect to energy cutoff

C. Additional Supporting Figures

The ground energy of the unit cell converges up to the 5th significant digit when with an energy cutoff surface of at least 500 eV. Hence, we conclude that calculations performed using $E_{cutoff} = 500$ eV or more are sufficient to model

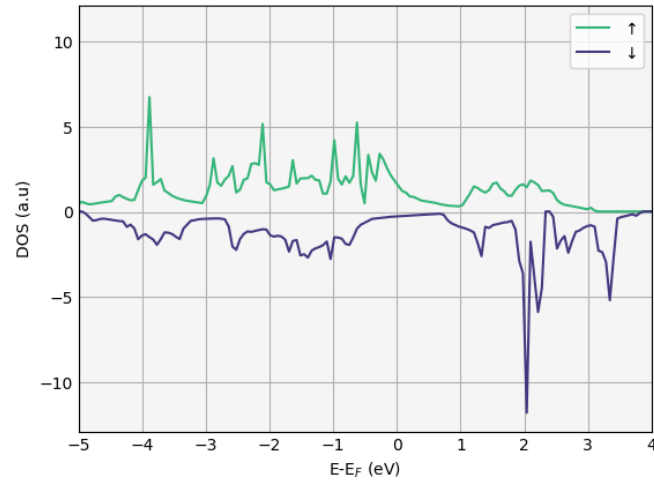


FIG. S2: DOS of the FM phase.

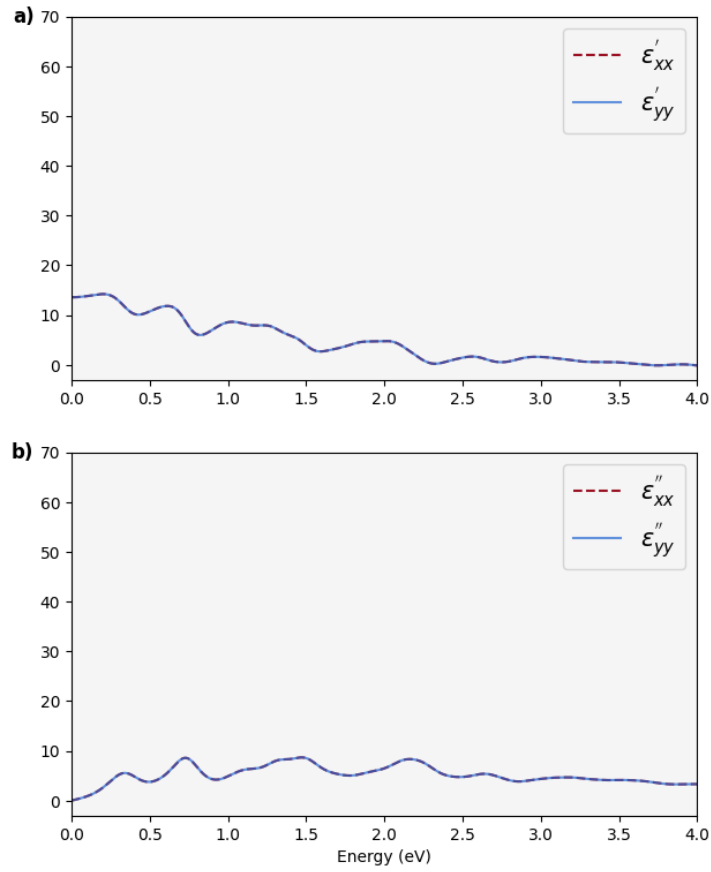


FIG. S3: Optical response of the FM unit cell along the x and y direction showing no anisotropy.

the behavior of the system.

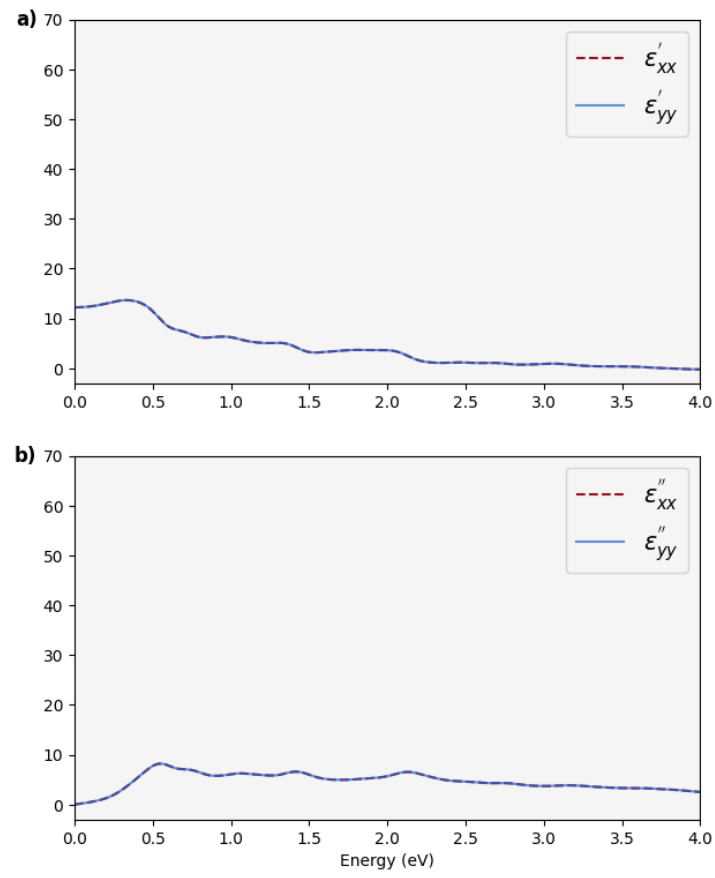


FIG. S4: Optical response of the FM-CDW supercell along the x and y direction showing no anisotropy.