Polarized Infrared Spectroscopy of $FeTe_2$ Single Crystals

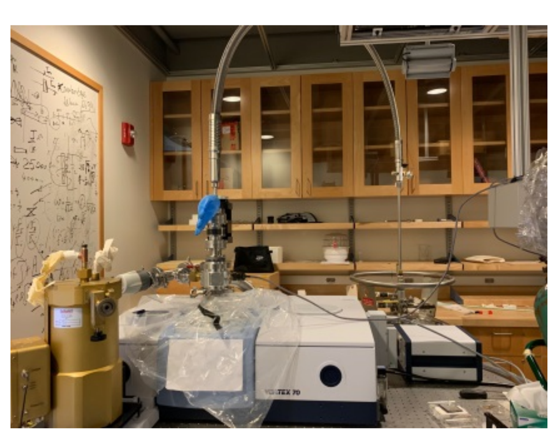
Prithivi Rana, Catalin Martin
Ramapo College of New Jersey, Mahwah, NJ, 07430

Introduction:

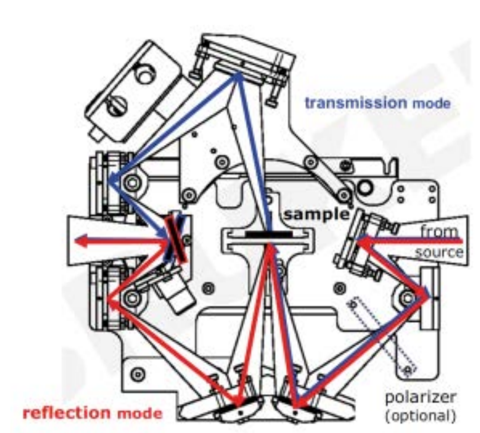
Initially studied for their thermoelectric properties, TMDs have garnered renewed interest for their potential in optoelectronic and spintronic devices. $FeTe_2$ is a promising TMD with recent reports predicting room temperature ferromagnetism. Some reports stated an absence of magnetic order in samples with iron vacancies. So, with the objective of answering some questions regarding their electronic properties, we performed optical measurements on samples with iron vacancies.

Method:

We performed polarized IR reflectance measurements: 0.04 – 6.2 eV(300 – 50,000 cm^{-1}) on a sample with mirror-like surface and < 0.5 mm diameter.



Bruker FTIR Vertex 70



R/T stage (≈ 11°)

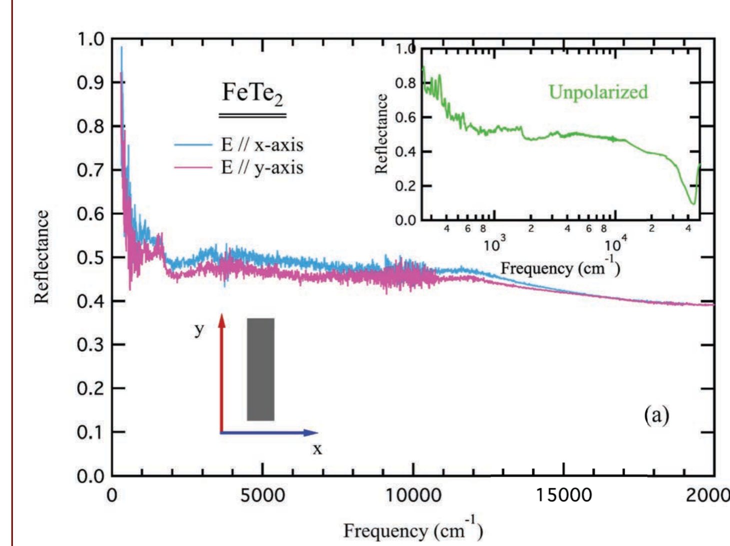
Reflectance:

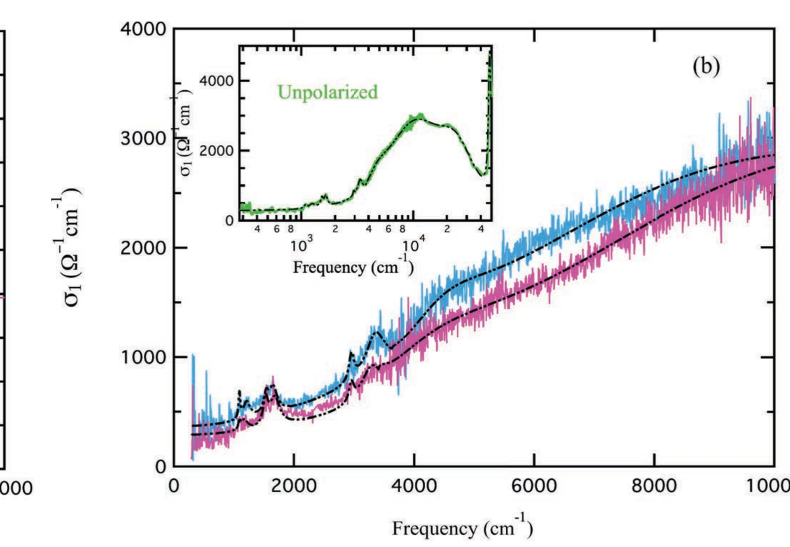
- Reflectance increases rapidly, reaching above 80% toward low frequencies (free carriers)
- Several sharp features at energies between 0.12 eV and 0.4 eV (significantly above those expected from phonon modes).
- Reflectance also shows a low anisotropy between the two polarizations (for almost the entire range).

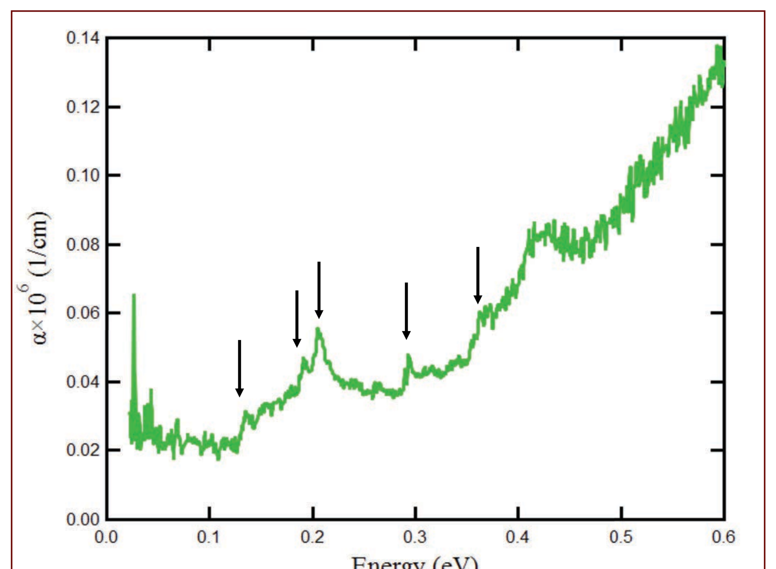
Optical Conductivity:

We achieved optical conductivity from Kramers Kronig transformation.

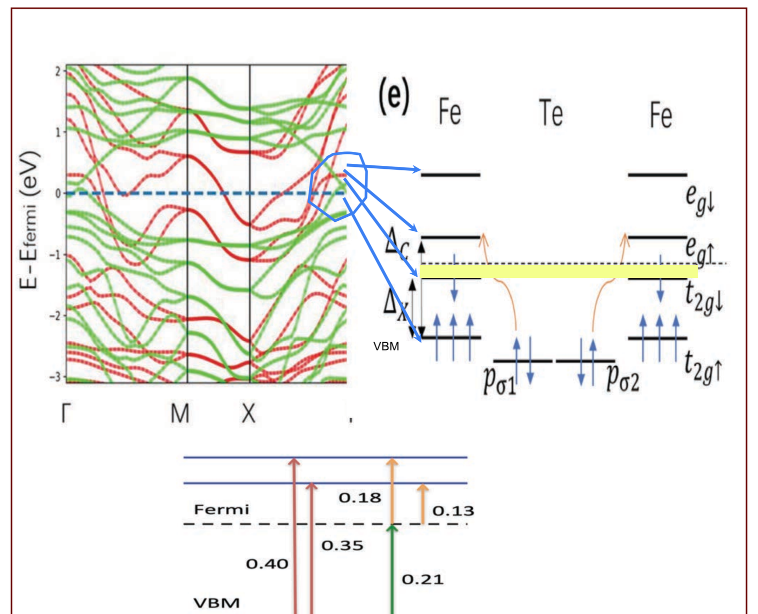
- Conductivity also shows anisotropy between the two polarizations
- Low but finite zero frequency conductivity
- Several sharp but weak features above 0.12 eV
- Strong absorptions at higher energies (onset at around 0.40 eV)







Additional optical transitions observed at low energies (below band gap
E_g ≈ 0.42 eV (↑↑ x axis)
E_g ≈ 0.47 eV (↑↑ y axis))



Spin splitting of the Fe 3*d* shell orbitals give rise to a band structure at the high-symmetry point

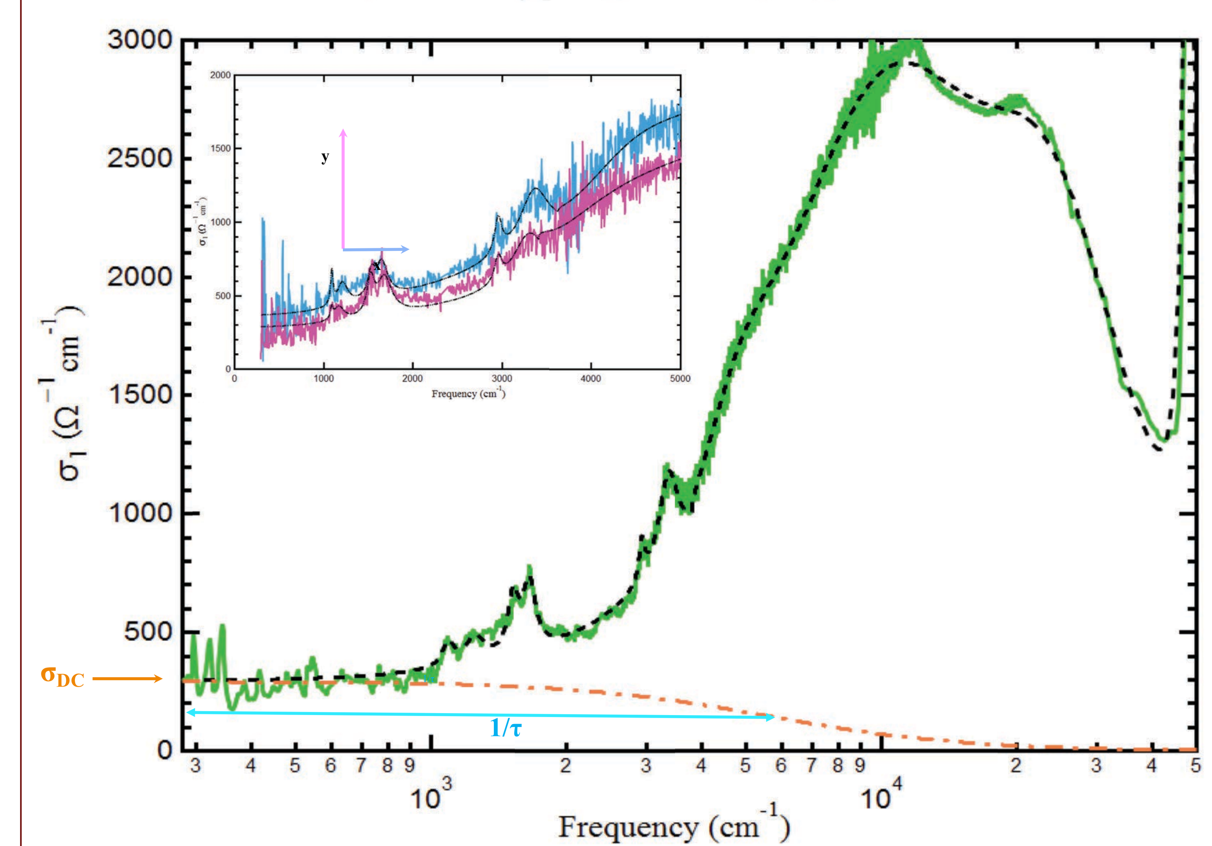
References:

- Tian, Jianjun, et al. **Physical Review B** 104, 224109 (2021)
- Liang Liu, et. al. **The Journal of Physical Chemistry Letters** 2020 11 (18), 7893-7900

Drude Conductivity:

We also include a Lorentz-Drude fit:

$$\tilde{\varepsilon}_r = \varepsilon_\infty - \frac{\omega_p}{\omega^2 + j\omega/\tau} + \sum_{i=1}^{N} \frac{\omega_{pe}^2}{\omega_{0i}^2 - \omega^2 - j\omega\gamma_i} \qquad \sigma_1 = \frac{\sigma_{DC}}{1+\omega^2\tau^2}$$



E// x-axis: σ_{DC} ≈ 370 Ω^{-1} cm^{-1}, 1/τ ≈ 0.8 eV
E// y-axis: σ_{DC} ≈ 290 Ω^{-1} cm^{-1} , 1/τ ≈ 0.7 eV

- Large values of 1/τ (0.01 – 0.02 eV in regular metals, Al, Cu, etc.)
- Anisotropy is given by different scattering rates.
- Good agreement with dc-transport data: σ_{DC} ≈ 400 Ω^{-1} cm^{-1}

Conclusion:

- Detected low in plane anisotropy of optical conductivity and optical band gap
- Agreement of our low energy optical absorption peaks with the energy levels involved in optical transitions
- Determined that there is a good match of our data with recent band structure calculations