CAN WE TEST QUANTUM FIELD THEORY ON MARS? A.J. Brown¹, P.C. Pinet², E. Cloutis³, A.M. Zastrow⁴, T.S.J. Gabriel⁵
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Introduction: A key aspect of our understanding of the world around us is the appreciation of the color of objects around us. The goal of this study is to perform a detailed study of the electronic spectra of a key mineral that is abundant on Mars, olivine.

We will use a Quantum Field Theory (QFT) [1] approach to model the spectra, including details such as temperature, composition (e.g. Mg-Fe-Mn) and structural parameters of olivine. We will compare and test the results of the code to the spectra from the VISIR SuperCam instrument, the CRISM orbital dataset, and laboratory spectra of olivine. We will also calculate the improvement of the QFT approach over the Crystal Field Theory (CFT) approach [2].

Methods: We will use a density functional theory ground state code, Quantum Espresso [3], coupled with a Bethe-Salpeter equation approach excitation code, yambo [4], to carry out the modeling to Hedin’s GW approximation [5]. These codes are based on the standard method of solving the Dyson-Bethe-Salpeter equation in a box for a large number of electrons. The models will provide the imaginary index of refraction of the electronic QFT spectral response.

We will then use the Shkuratov approach [6] to calculate grain sizes from the optical constants produced by the QFT models. This model has been shown to give consistent results, and is based on deriving the reflected properties of a stack of plates of the required optical properties.

We will also use a Kramers-Kronig approach to derive the real part of the optical response from the absorption part of the spectrum [7]. This will be used as necessary to compare to the perceived color of the olivine mineral.

SuperCam: SuperCam is a multi-instrument suite on the Mars2020 rover equipped with Optical, Raman and LIBS instruments [8]. We will use the SuperCam VISIR data set which covers the relevant region of the electronic excitations and has collected spectra of olivine rich targets at its landing site at Jezero Crater [9].

CRISM: We have will use orbital (CRISM) data to examine spectra from the olivine-rich lithology in the CRISM HRL40FF image over Jezero Crater at the MTRDR level of atmospheric correction [10]. Figure 2 shows an example of the olivine spectrum from this image. This spectrum shows the relatively deep olivine absorption band in the 0.6-1.9 μm region. A central challenge to this work will be that material mixtures within the surface and orbital field of view can cause some deviations from first principles. However, these olivine features are some of the most pristine available for Mars.

Fig. 2. CRISM spectrum of Olivine band in the margin unit, from HRL40FF over Jezero crater in pixel coordinates at x=258, y=479. Dataset available at this PDS link.

Fig. 1. Olivine lattice structure, showing the M1 and M2 sites for Mg and Fe substitution and octahedral splitting of the 3d transition electrons under Crystal Field Theory [2].
Laboratory work: We will also test the QFT model results against the recent laboratory spectroscopy of olivine with varying composition of Pinet et al. [11] and measured at the HOSERLab [12]. The variable composition is critical to the testing of the QFT model which can be prepared with any mafic ion.

Asymmetric modeling: We will use an asymmetric Gaussian modeling approach [13] to map the electronic bands and compare them with previous work which was able to constrain the Jezero region olivine to a Fo# between 45-66 [14]. Figure 3 shows an example of the asymmetric Gaussian modeling approach.

Figure 3 (A) demonstrates one method of mapping two overlapping absorption spectra. In this approach, we have calculated the difficulty of correctly discriminating between the overlapping Gaussian spectral bands as they pass through each other. The left part of the figure shows that the difficulty increases as the centroids get close to each other, but also as the widths of the Gaussian gets narrower. Figure 3 (B) shows two overlapping spectra in brown and their derivatives in blue.

We will use these insights into developing an automated overlapping Gaussian routine because the olivine bands in the visible region of the spectrum is actually a 3 or 4 band complex [11,15], and this will require special techniques to account for the discrimination of individual bands from Mars spectra, to compare them to QFT calculations.

CFT results. In Table 1 we present a subset of the CFT results from Burns Table 5.5 [2]. We will use these data points in our first comparisons. Table 5.5 of Burns also includes the results for Ni and Mn cation substitution, allowing us easy access to those cations as we move forward.

<table>
<thead>
<tr>
<th>Fo-Fa# (xFe)</th>
<th>Site</th>
<th>Band center (cm$^{-1}$)</th>
<th>$\Delta_0$ param (cm$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.08-0.98</td>
<td>M1</td>
<td>9090-8060; 11830-11050</td>
<td>9670-8830</td>
</tr>
<tr>
<td></td>
<td>M2</td>
<td>9570-9280</td>
<td>8210-7930</td>
</tr>
</tbody>
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Table 1. Olivine electronic bands for forsterite-fayalite series

Take away messages: We are developing a process for understanding Mars surface and orbital olivine spectra using QFT and CFT.

We intend to use the variations in composition, temperature and grain size to compare with the Martian olivine spectra by CRISM, SuperCam and in the laboratory.

This is the first report on this approach and we anticipate future work in this area will enhance our understanding of the linkages between the color of minerals as measured from remote sensing platforms and their composition.