*Ab Initio* Calculated Reflectance Spectra At Room And High Temperature Of Mg-Silicates Of Mercury Surface: A Tool To Interpret Thermal Ir Emissivity Spectra Acquired In Remote Sensing. C. Stangarone¹, J. Helbert², A. Maturilli², M. D’Amore², S. Ferrari², M. Tribaudino¹, M. Prencipe³, ¹Physics and Earth Science Department, University of Parma, Viale G P Usberti, 7/A, 43125, Parma, Italy (claudia.stangarone@studenti.unipr.it), ²Institute for Planetary Research, DLR, Rutherfordstrasse 2, 12489 Berlin, Germany, ³Earth Science Department, University of Turin, Via Valperga Calusco, 35, 10125 Torino, Italy

**Introduction:** Spectral signatures of minerals are intimately related to the crystal structure; therefore they may represent a remote sensing model to determine surface composition of planetary bodies, by analysing their spectral reflectance and emission collected in remote sensing. However, one of the most critical point is data interpretation considering planetary surfaces, especially Mercury, where changes in spectral characteristics are induced by the high temperatures conditions [1]. The aim of this work is to interpret the experimental thermal emissivity spectra with an innovative approach: simulating IR spectra of the main mineral families that presumably compose the surface of Mercury and compare them to high temperature laboratory measurements. In this work we are focusing on Mg-pyroxenes and Mg-olivine [2], both at room and high temperature, exploiting the accuracy of *ab initio* quantum mechanical calculations, by means of CRYSTAL14 code [3]. Results will be useful to create a theoretical background to interpret high temperature infrared (HT-IR) emissivity spectra that will be collected by the Mercury Radiometer and Thermal infrared Imaging Spectrometer (MERTIS), the spectrometer developed by DLR that will be on board of the ESA BepiColombo Mercury Planetary Orbiter (MPO) [4]. As a first goal we mean to understand which IR frequencies are influenced by temperature that occurs during the insolation of the surface and which not, after a.

**Computational details:** The IR reflectance spectra of orthoenstatite and forsterite end members have been simulated first at ambient condition, using the Hybrid HF/DFT Hamiltonian WC1LYP, by means of CRYSTAL14, a computational program for *ab initio* methods, which employs localized, gaussian- type basis sets. The chosen Hamiltonian was WC1LYP which is based on the Wu-Cohen exchange functional [5], corrected by a fraction (16%) of non-local exact Hartree-Fock exchange, and Lee-Young-Parr correlation [6]. The reflectance spectra have been simulated by computing the dielectric susceptibility tensors up to the third order, by means of (CPHF/KS) method. With such a method it is also possible to compute the LOTO splitting, and hence to simulate reflectance oriented IR spectra of orthoenstatite along the x, y and z directions. IR vibrational frequencies has been performed also from 0K to 100K, in order to simulate Mercury extreme environment conditions.

High temperature calculations are performed evaluating the vibrational frequencies at the unit cell at different volumes, as a consequence of an increasing range of temperature. IR frequencies and intensity has been calculated for volume estimated at 0 and 1000K (extreme situations) taking into account zero point Energy.

**Experimental details:** At Planetary Emissivity Laboratory (PEL) [1,7] emissivity and reflectance measurements have been performed to identify mineral structures in the IR spectral region between 50 and 1400 cm⁻¹. Within this range, silicates have a unique set of spectral absorption features that allow them to be distinguished from each other [8]. PEL is currently equipped with two Fourier transform evacuable Bruker Vertex 80V spectrometers. One of them is connected to a planetary simulation chamber, that has the unique capability to heat samples to temperatures up to 1000K. The samples that have been measured are 1) orthoenstatite, from Bamble, Norway, with chemical composition (Mg0.85Fe0.15)2Si2O6 and a forsterite with chemical composition Mg1.84Fe0.16SiO4. Measures have been performed on four different grain sizes (0-25µm; 25-63 µm; 63-125 µm; 125-250 µm), to study the effect due to volume scattering of particles.

IR reflectance measurements have been performed at room temperature in vacuum. For the analysis 0.3 grams of material are required. Emissivity measurements are performed at different temperatures, from 320K up to 1000K, with T steps of 100K. For these measures we need more material (from 3 to 4 grams each size separate) and since they take longer in terms of time for each T step and calibration, we analized only the finer and the coarser grain sizes.

**Comparison and outlooks:** Here we report a first qualitative comparison between calculated reflectance spectra and experimental measures of orthoenstatitte. The experimental spectra is the coarsest grain size sample. The calculated spectra is the weighted arithmetic mean of the three calculated oriented spectra x y z. A very good agreement appears, especially within the region 700-1400 cm⁻¹, which will be the part of the region acquired by MERTIS [4]. Data processing and comparisons with calculated data are in progress. Experimental data from thermal emissivity measurements with IR vibrational frequencies calculated at HT, will
be compared to check if the predicted frequencies shift with temperature is in agreement with experimental emissivity band shifts.

Figure 1: Comparison between calculated reflectance spectra and experimental measures of orthoenstatite at room temperature. The calculated spectra is the weighted arithmetic mean of the three calculated oriented spectra x y z.