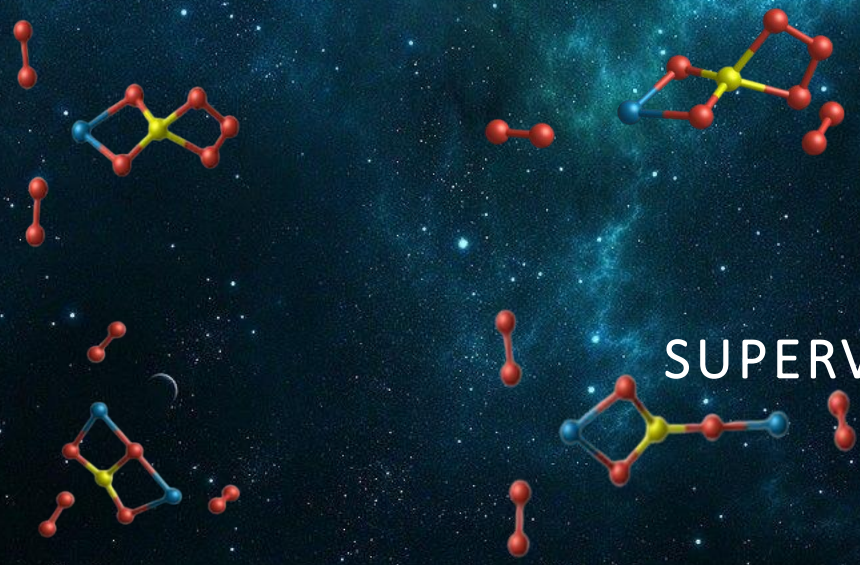
UNIVERSITAT DE BARCELONA

Institut de Química Teòrica i Computacional
UNIVERSITAT DE BARCELONA

EXCELENCIA MARÍA DE MAEZTU

Nanoclusters & Nanostructured Materials

NANOSILICATE CLUSTERS AND THEIR INTERACTION WITH OXYGEN: ASTRONOMICAL RELEVANCE



JOAN MARIÑOSO GUIU

SUPERVISOR: STEFAN T. BROMLEY

IBER 2023

SEPTEMBER 2023

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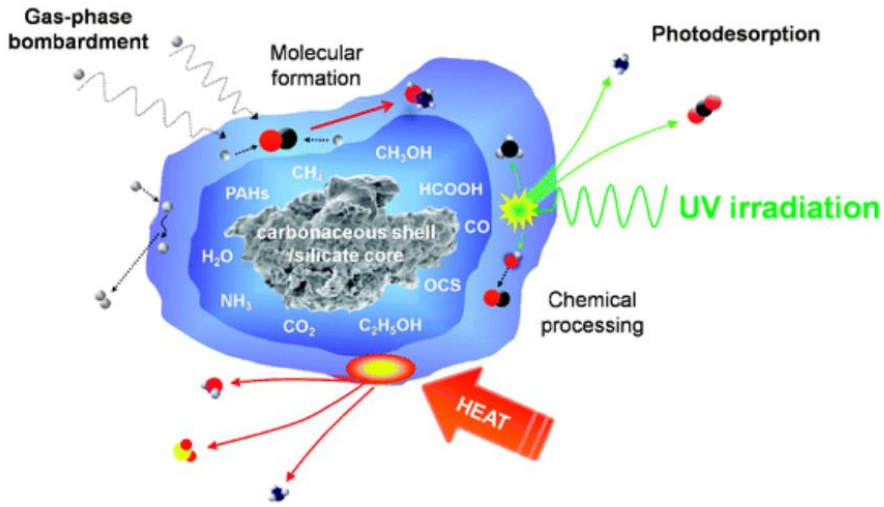

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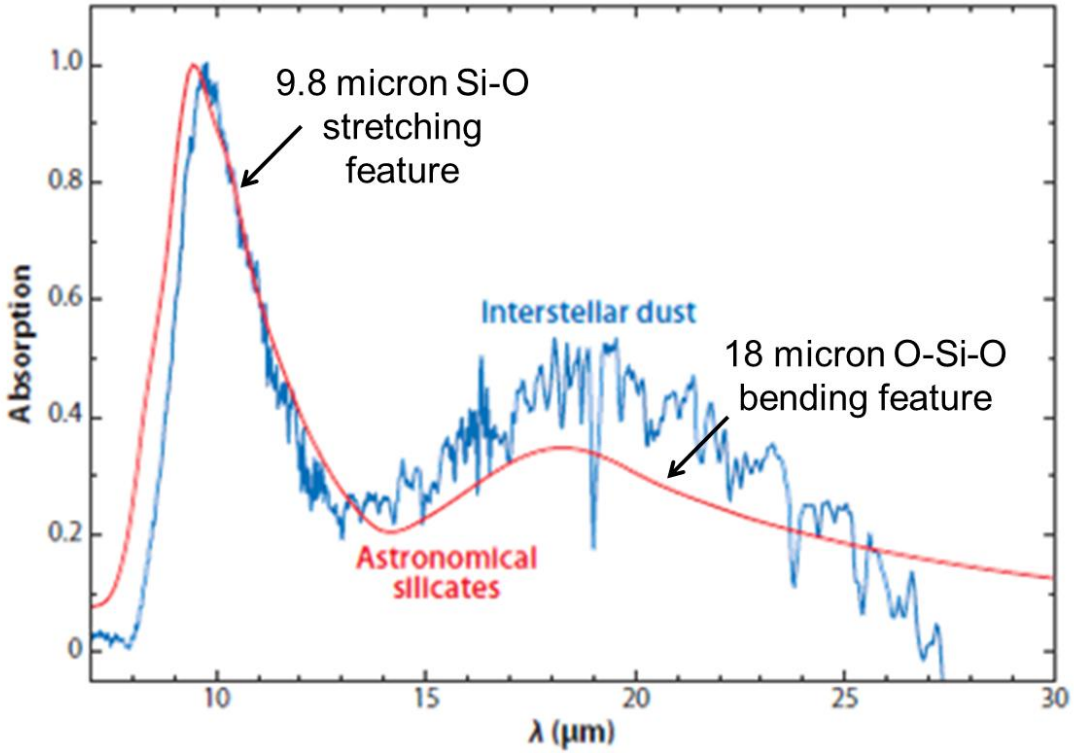

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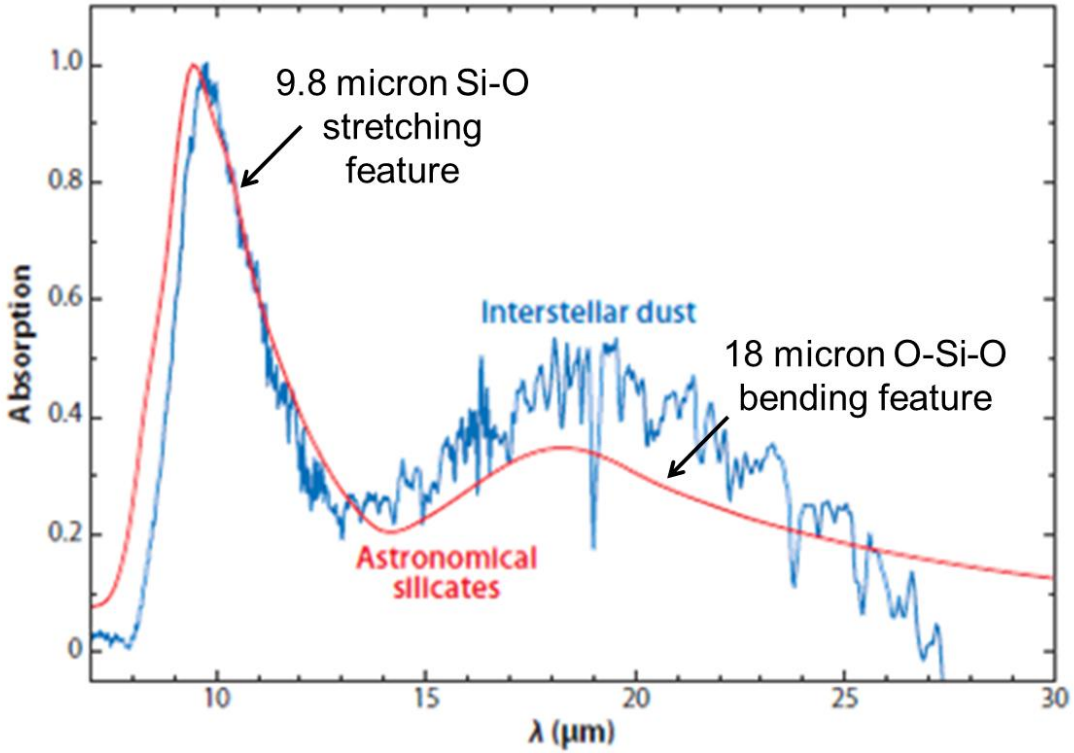
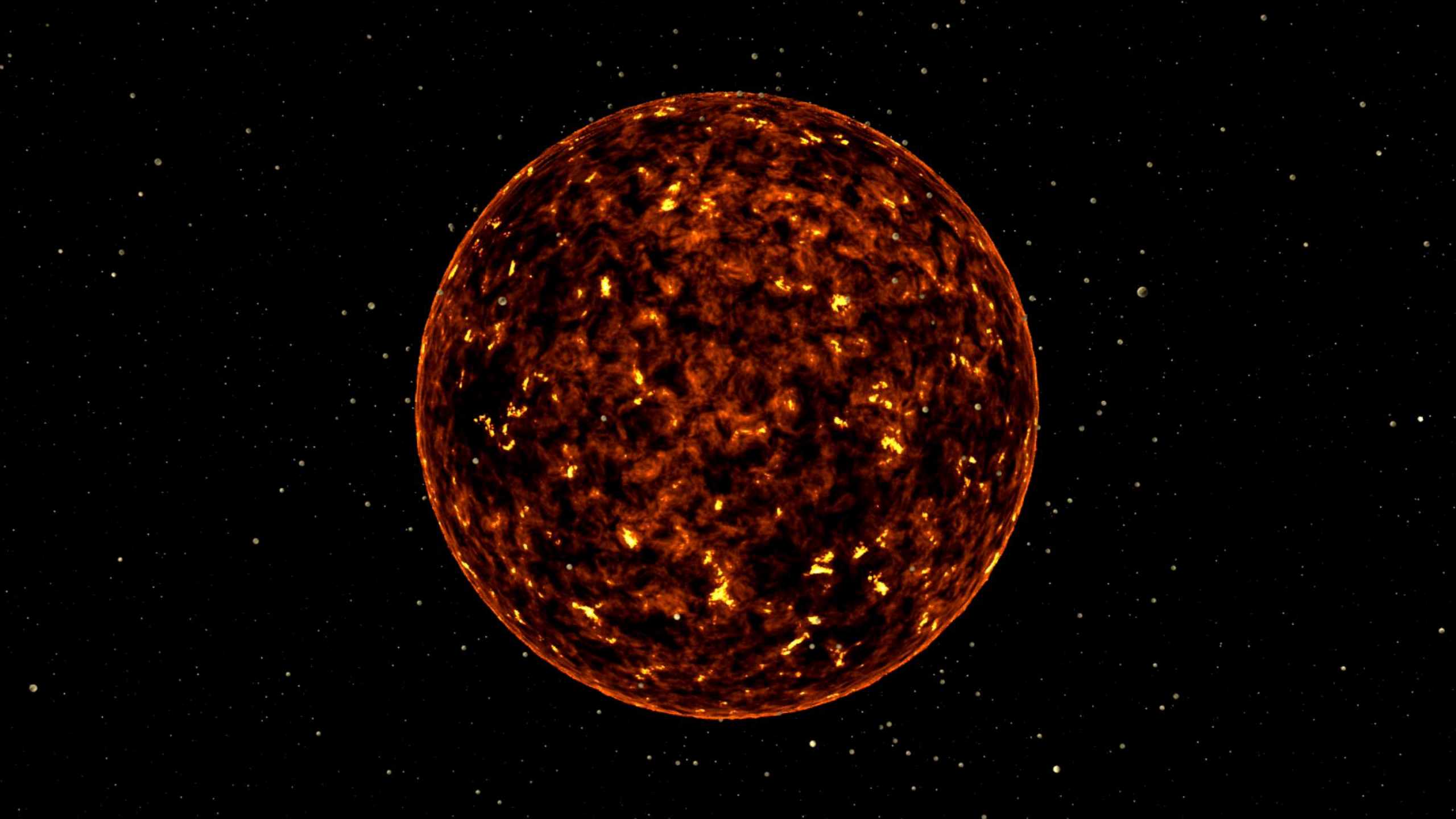
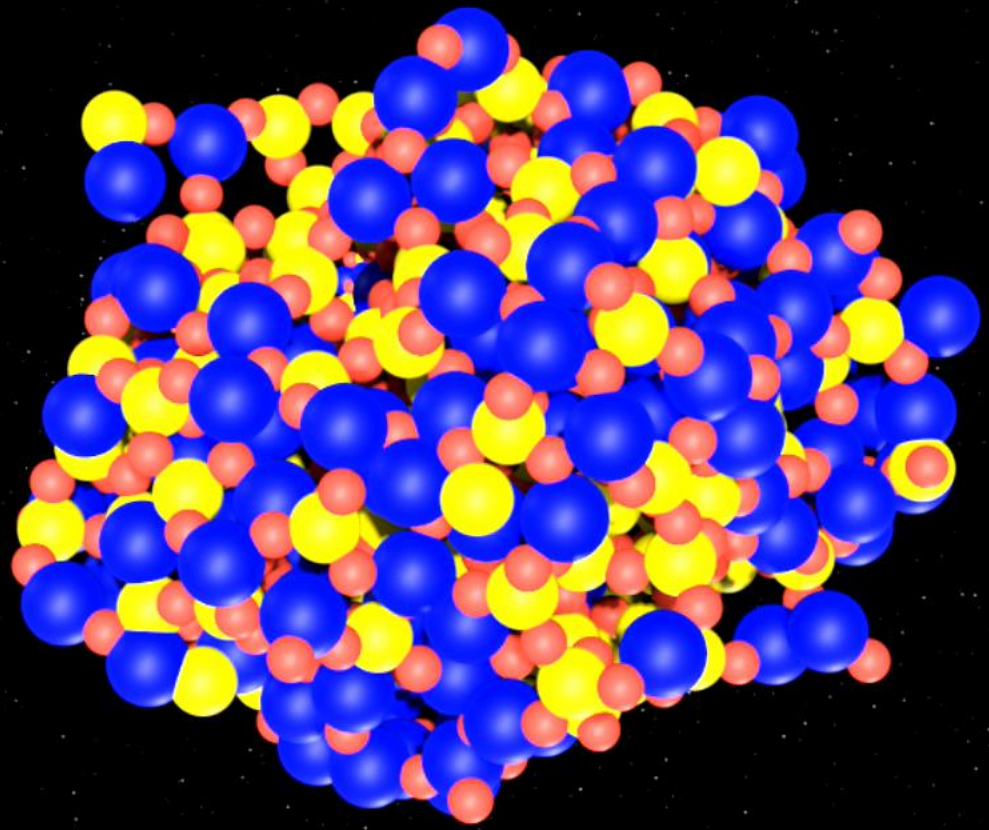
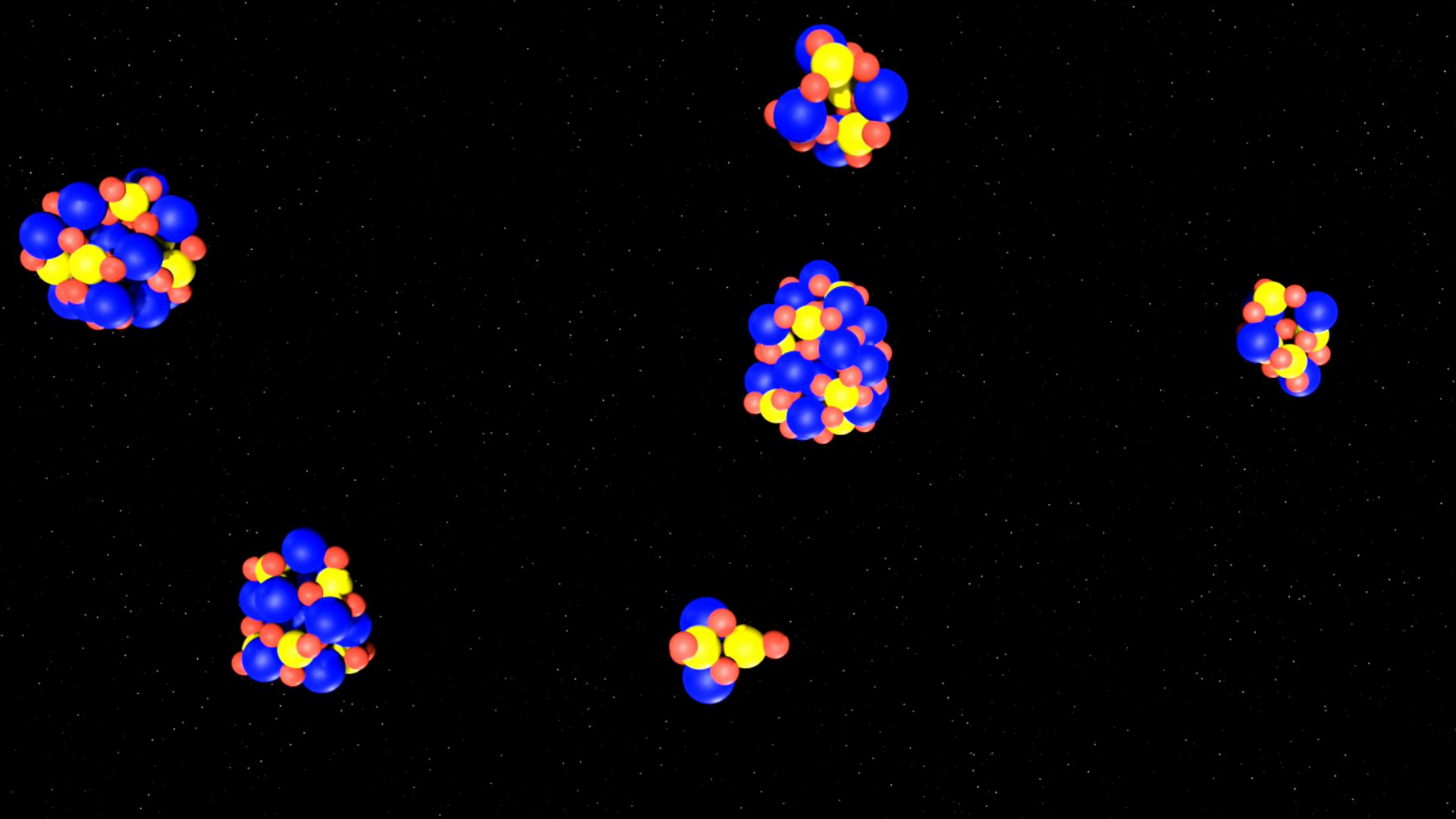


WHERE ARE SILICATES FORMED IN SPACE?







WE HAVE MODELS FOR NANOSILICATES

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Joan Mariñoso Guiu, Antoni Macià Escatllar, and Stefan T. Bromley*

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Published as part of The Journal of Physical Chemistry virtual special issue "10 Years of the ACS PHYS Astrochemistry Subdivision".

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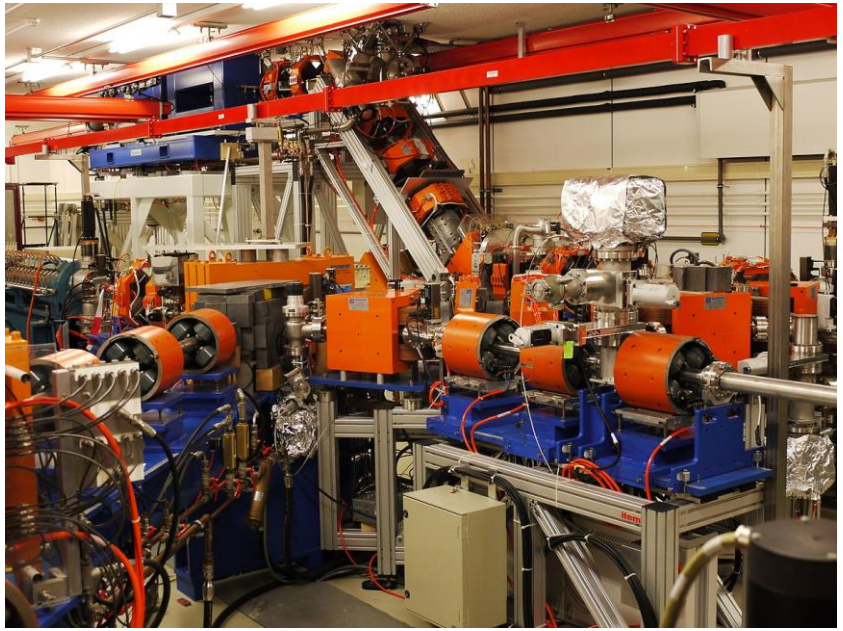
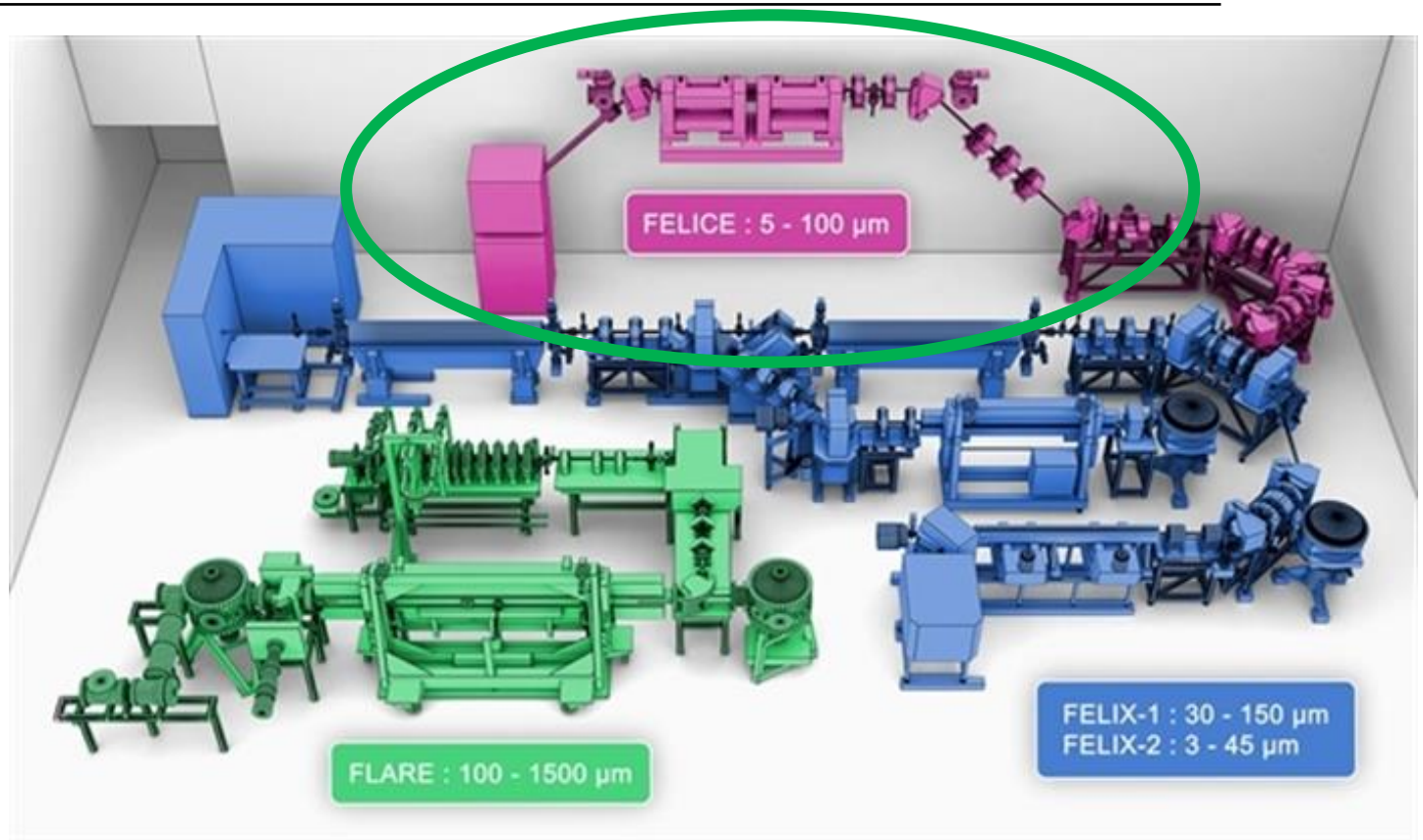
EXPERIMENTAL COLLABORATORS!

EXPERIMENTAL SET-UP



FELIX

Free Electron Lasers for Infrared eXperiments



Free **E**lectron **L**aser for **I**ntra **C**avity **E**xperiments

EXPERIMENTAL RESULTS

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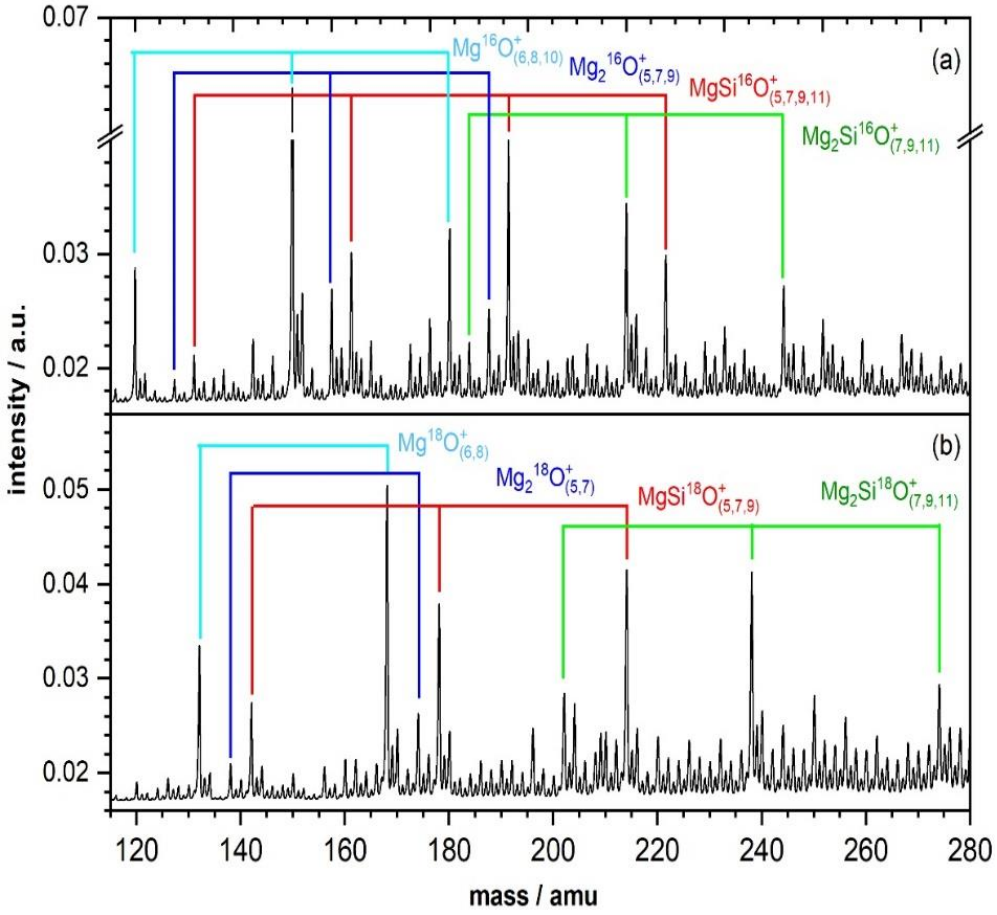
$MgSiO_9^+$ **$Mg_2SiO_9^+$**



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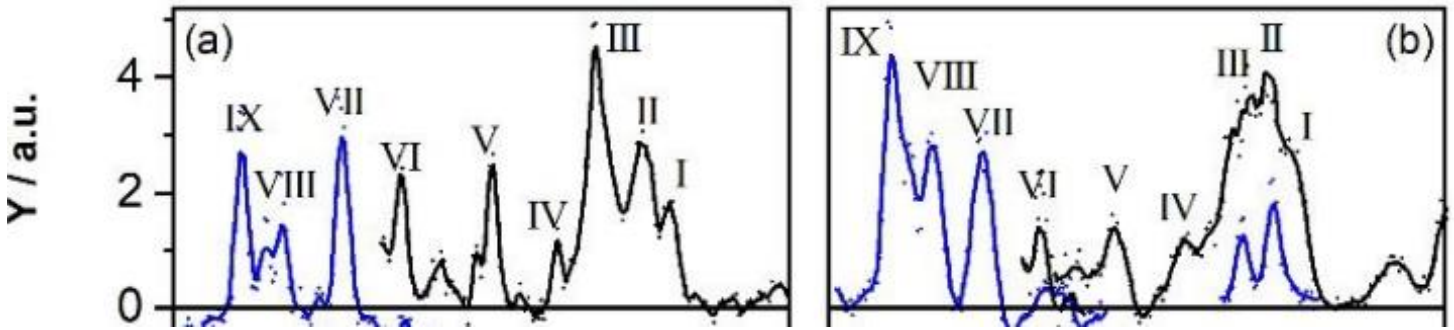
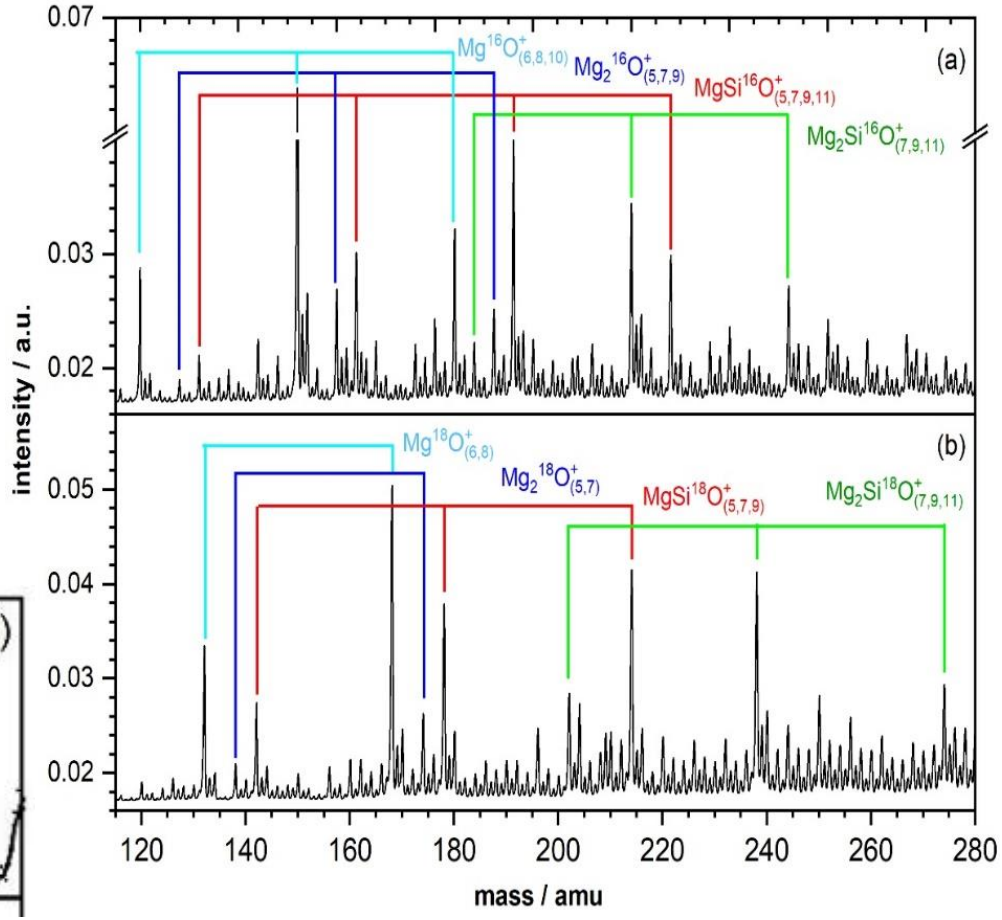
  $MgSiO_9^+$ **$Mg_2SiO_9^+$**
- Obtained the IR spectra of the clusters.





TIME TO MODEL NANOSILICATES

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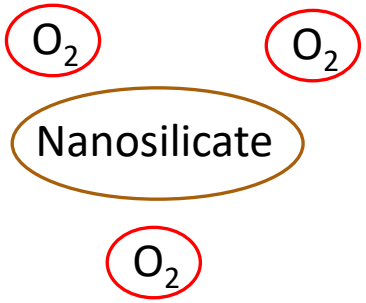
- Assume cationic silicate core interacting with oxygen molecules.



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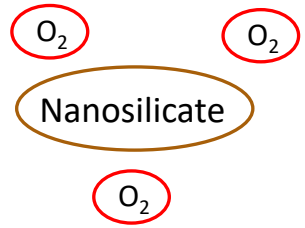

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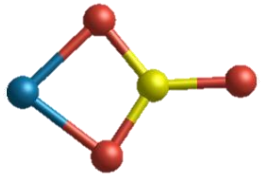

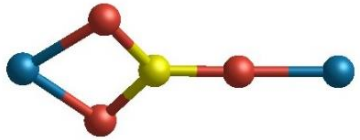

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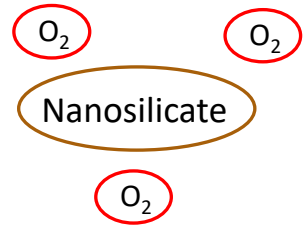

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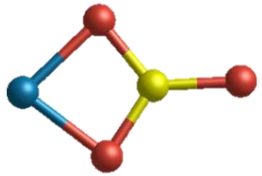
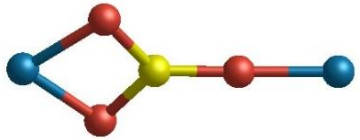


- Refinement of the structures using DFT-PBE0.

PBE0 good for IR spectra compared with high level of theory data[1]

FHI-aims
The ab initio materials simulation package

[1] *ACS Earth Space Chem.* 2021, 5, 4, 812−823

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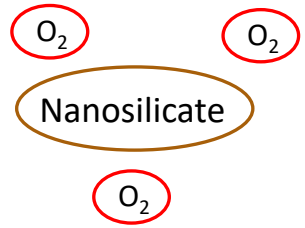

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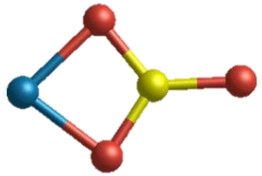
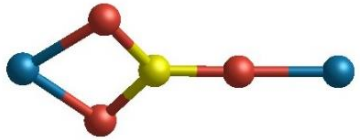


O Mg Si

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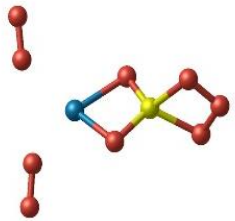
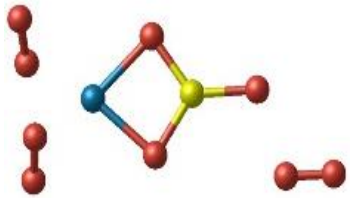
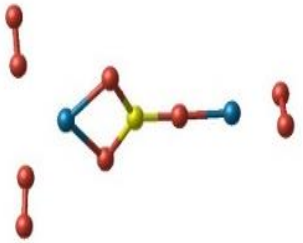
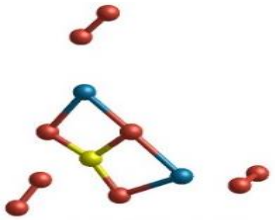
- Systematic sampled positions of the oxygen molecules.

Dispersive non-bonded interactions included (TS method)

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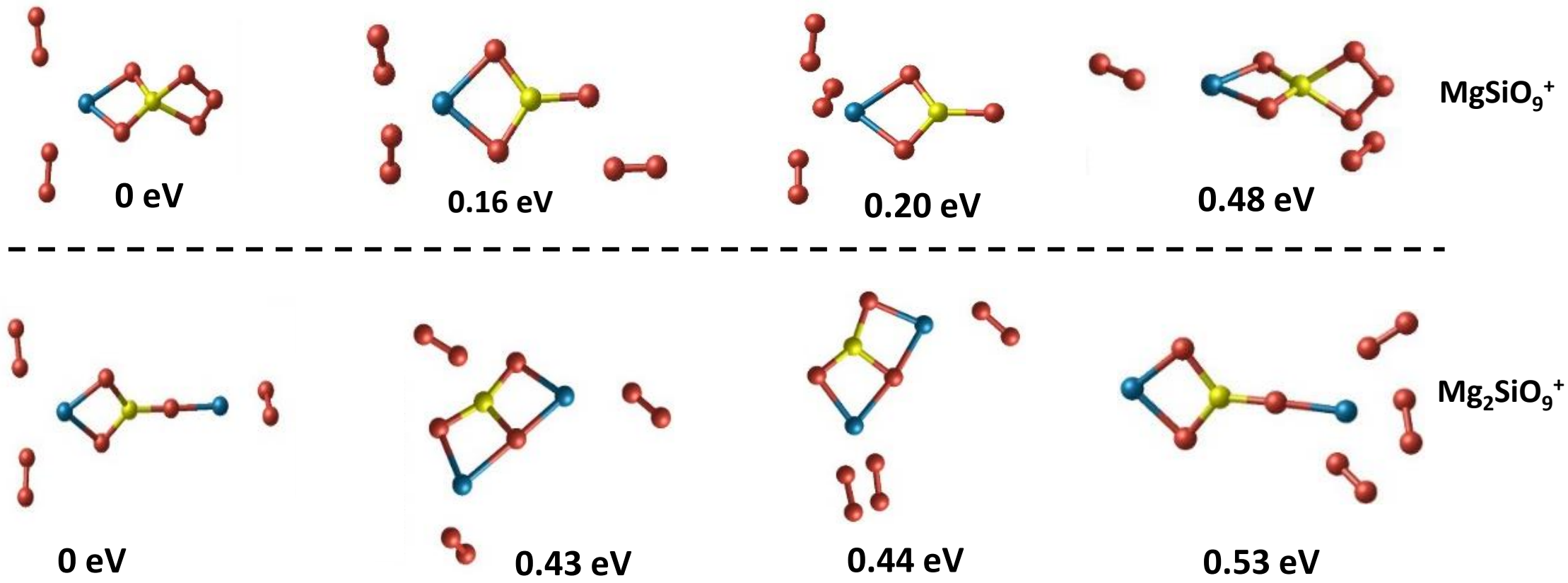

MOST STABLE ISOMERS FOUND

WHAT DO WE HAVE SO FAR?

EXPERIMENTS

MODELS

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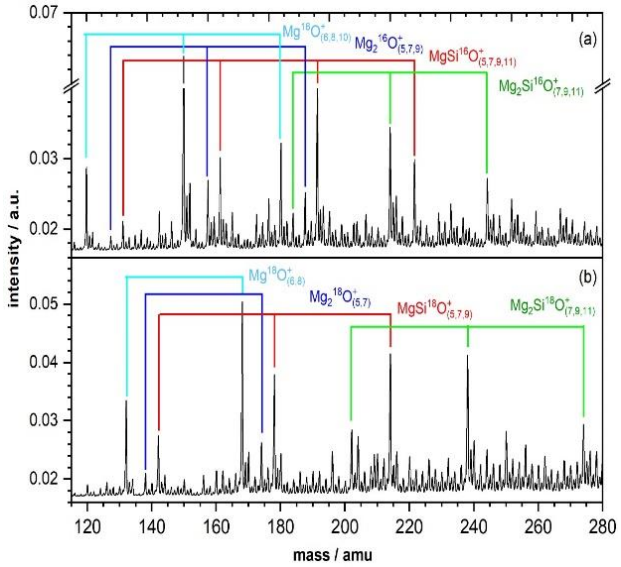

Stoichiometry determination

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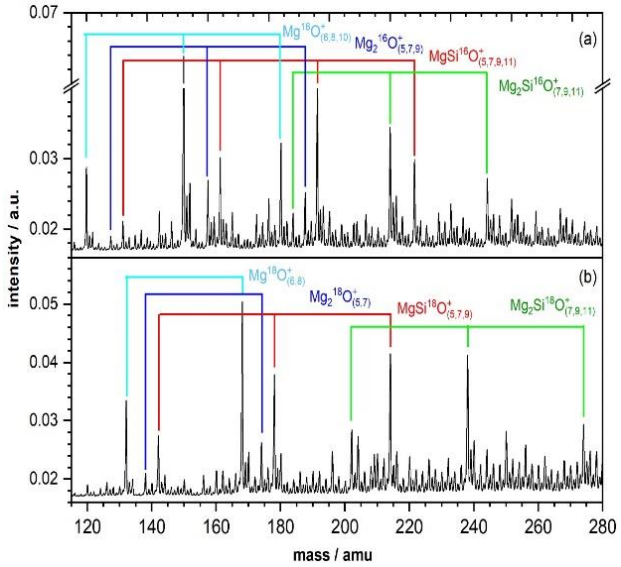

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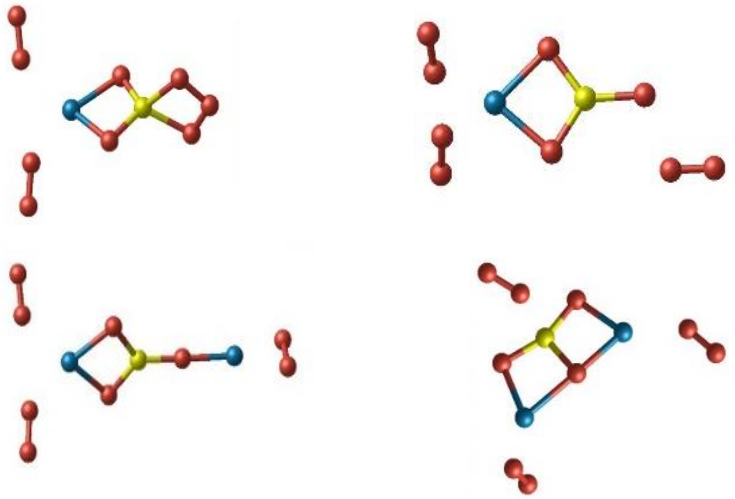

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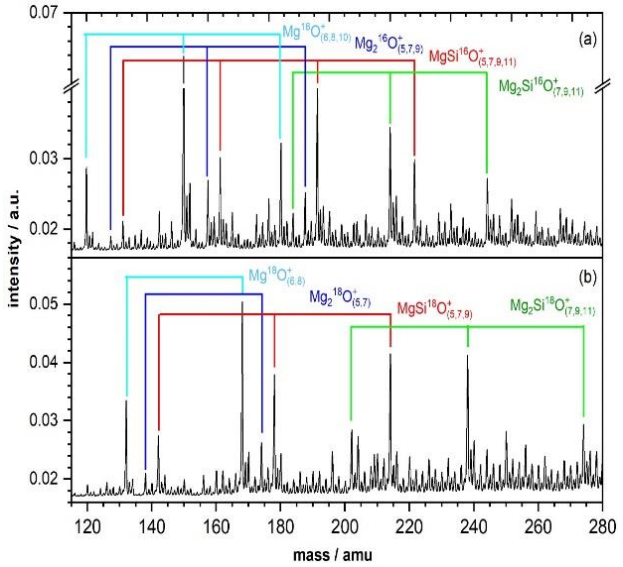

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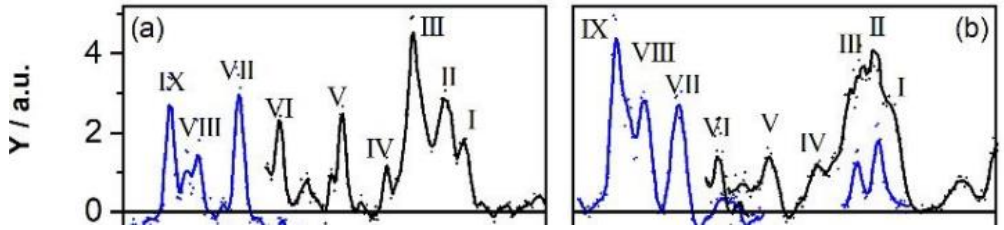
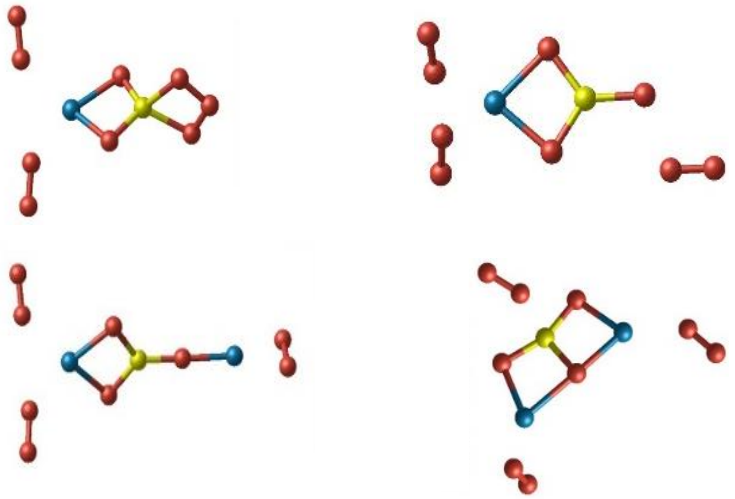


IR spectra

MODELS



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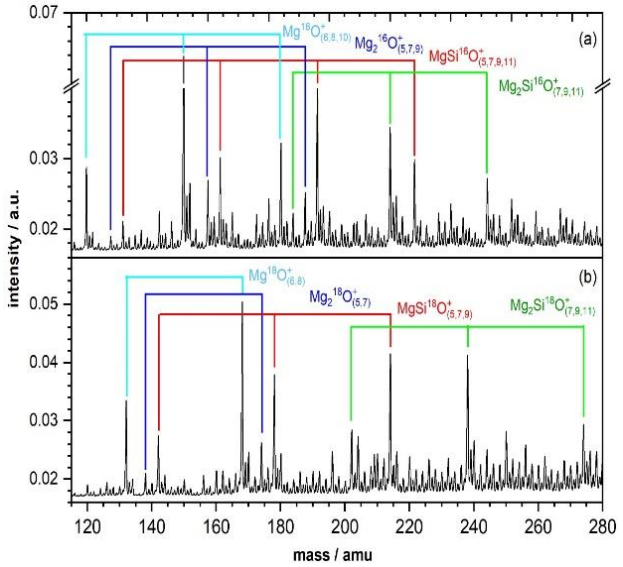

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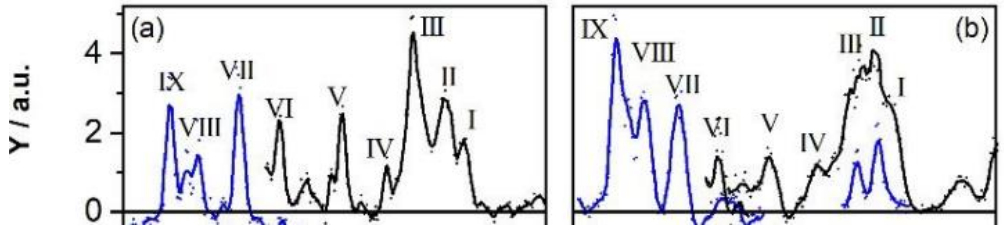

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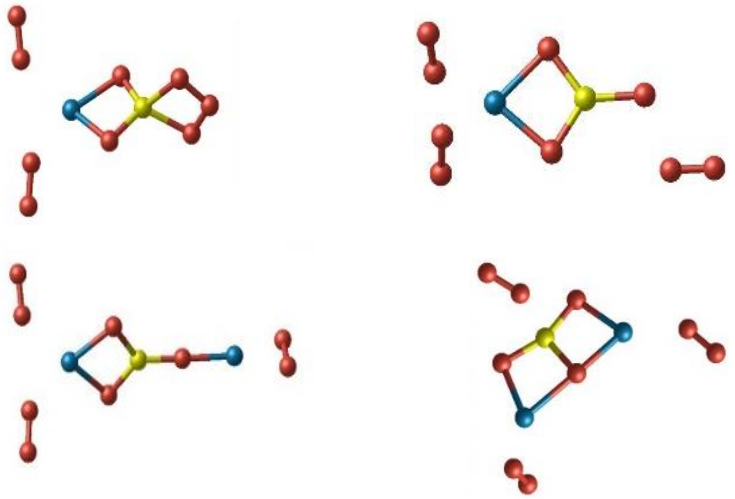
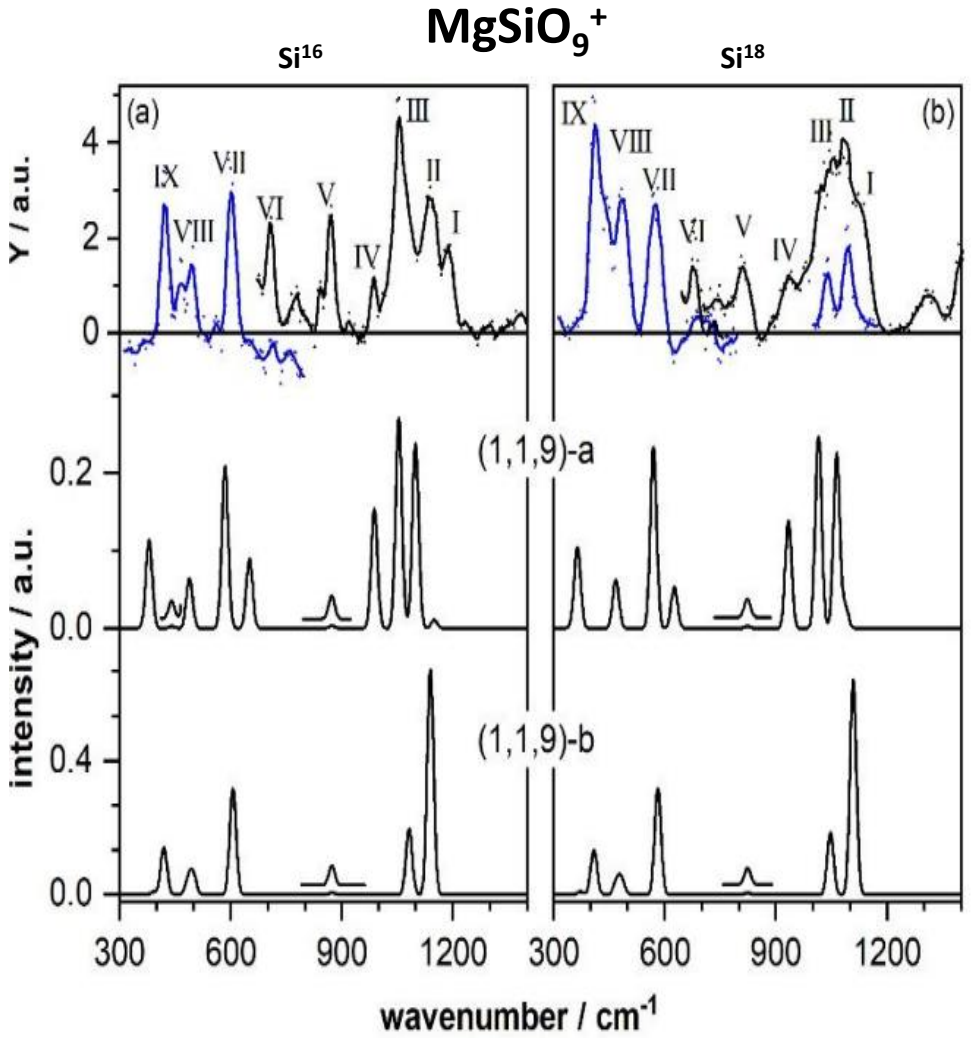


COMPUTATIONAL SPECTRA
TO CONFIRM MODELS

COMPARE IR SPECTRA



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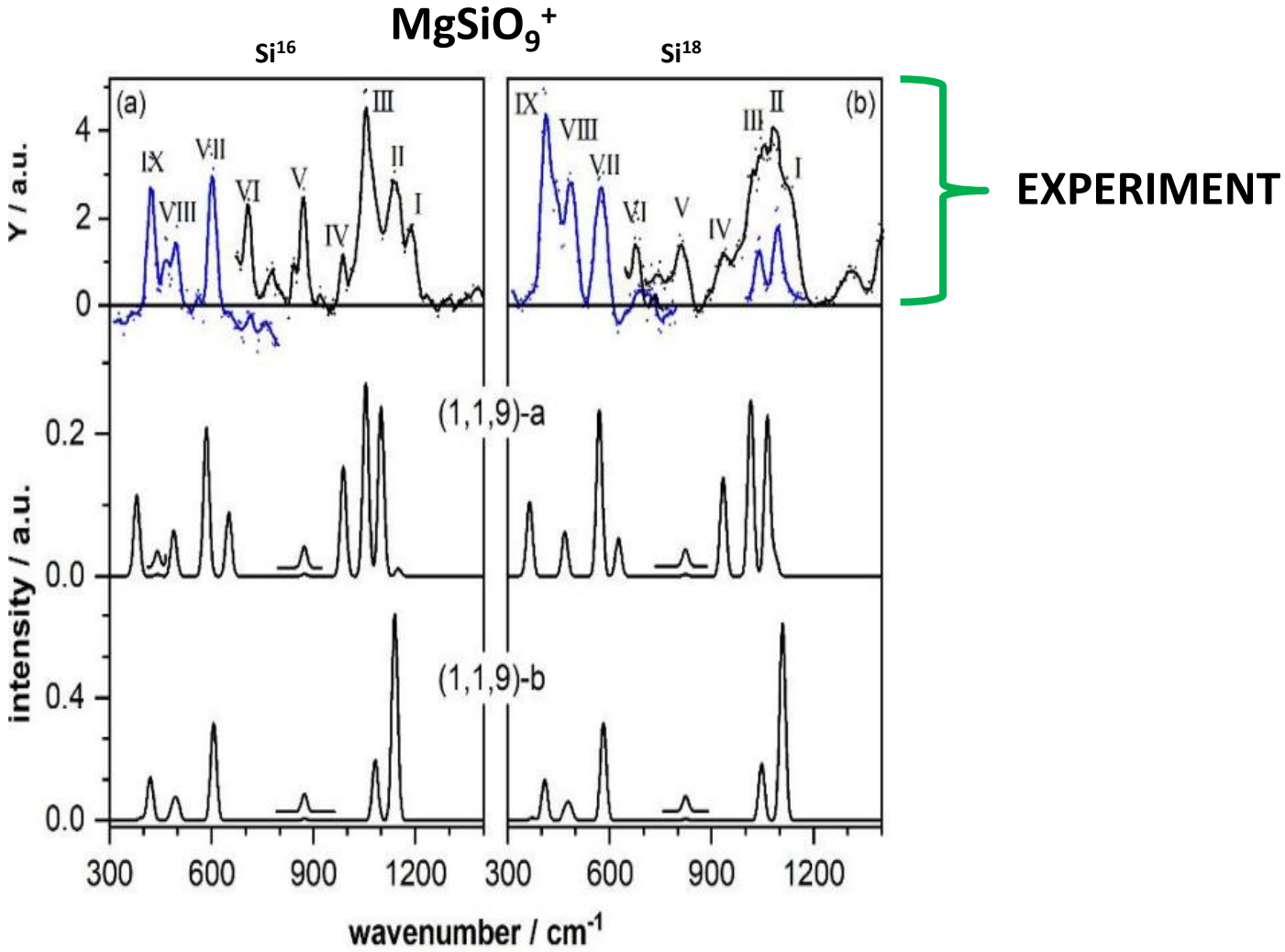

EXPERIMENT

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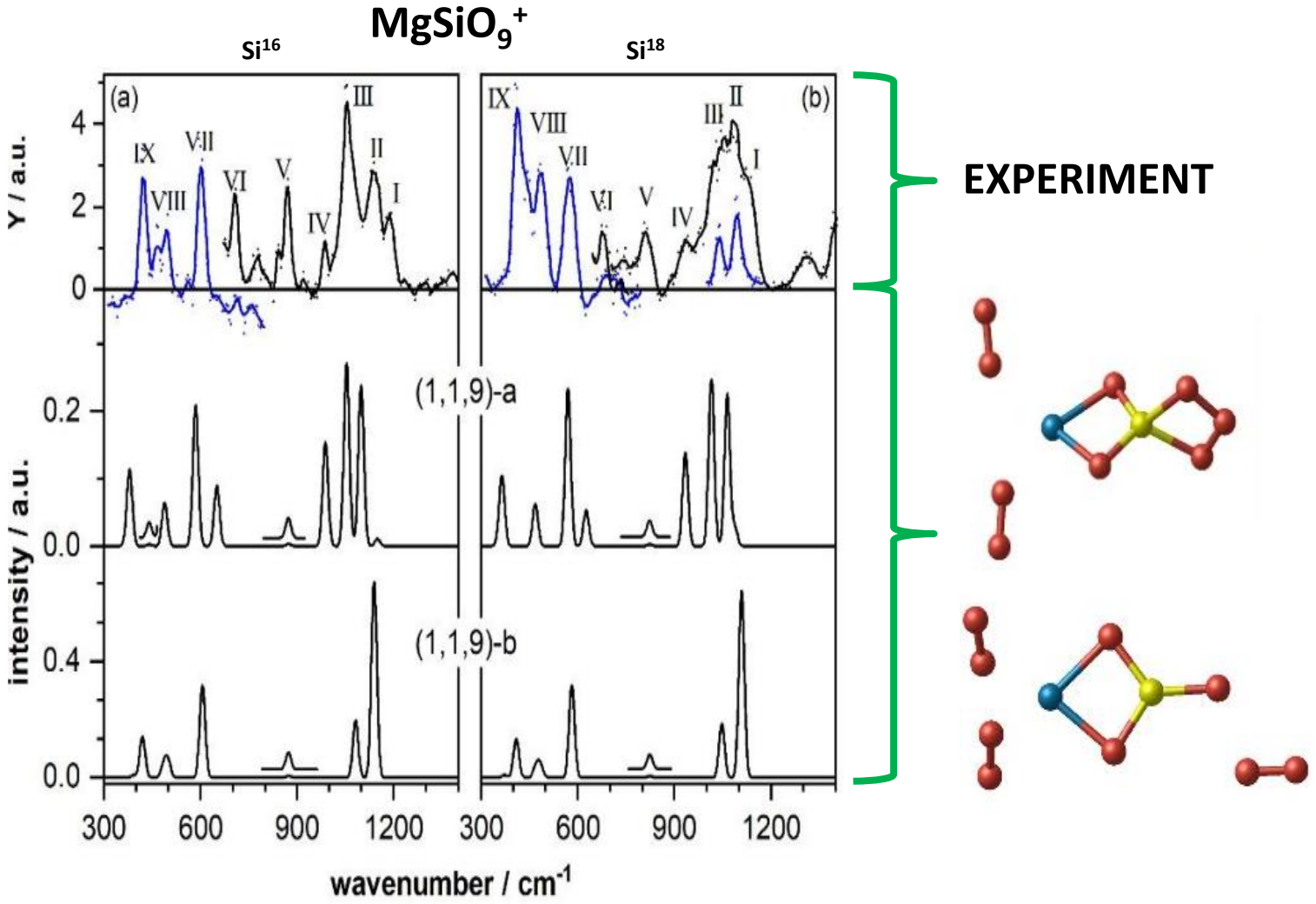

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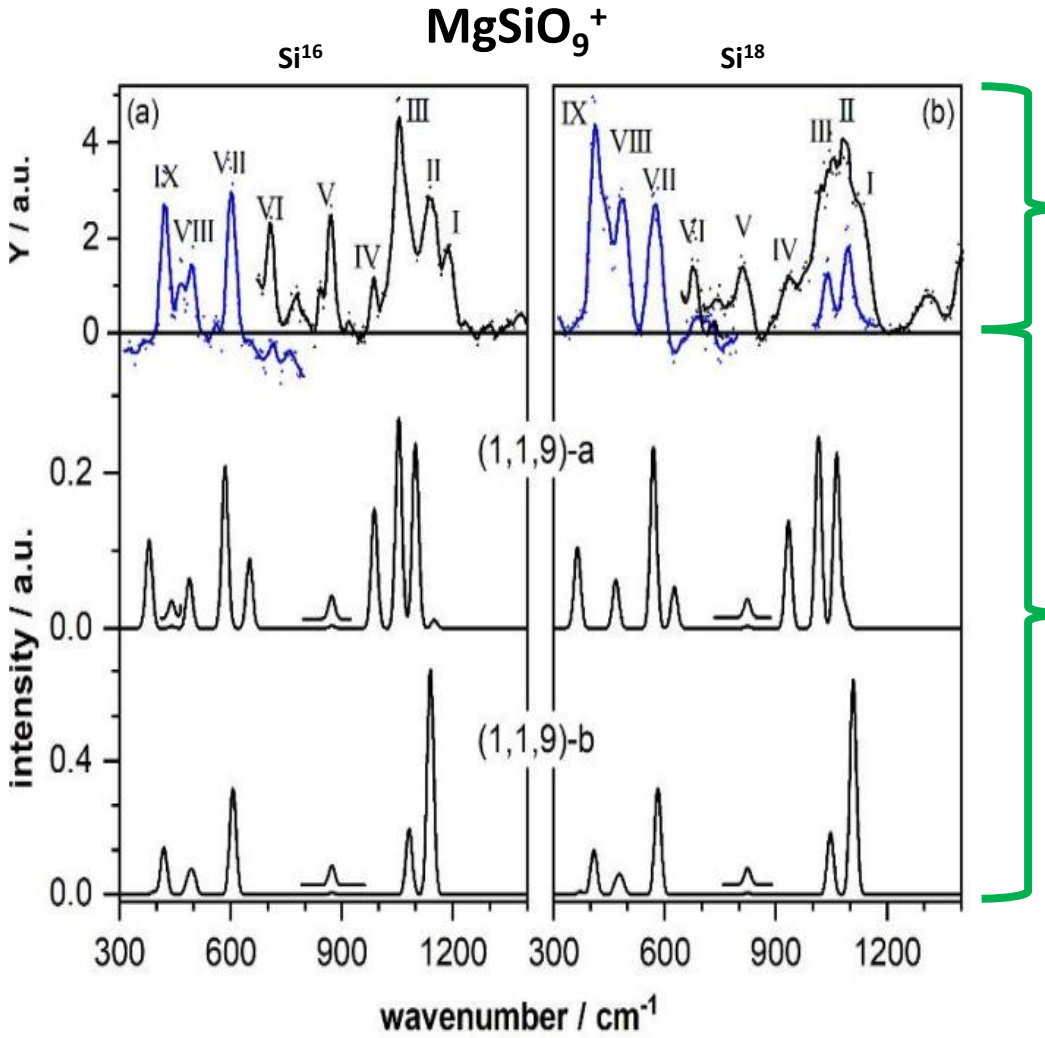

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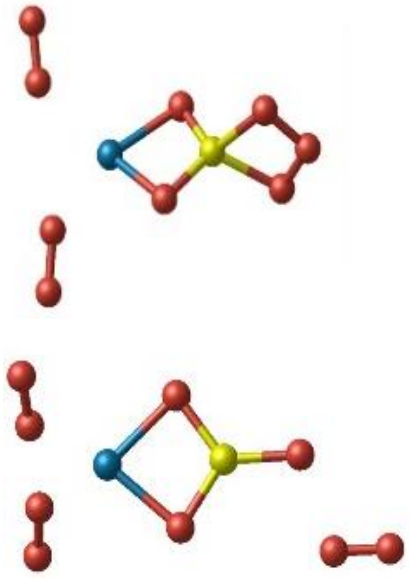

- Good agreement between experiment and models.

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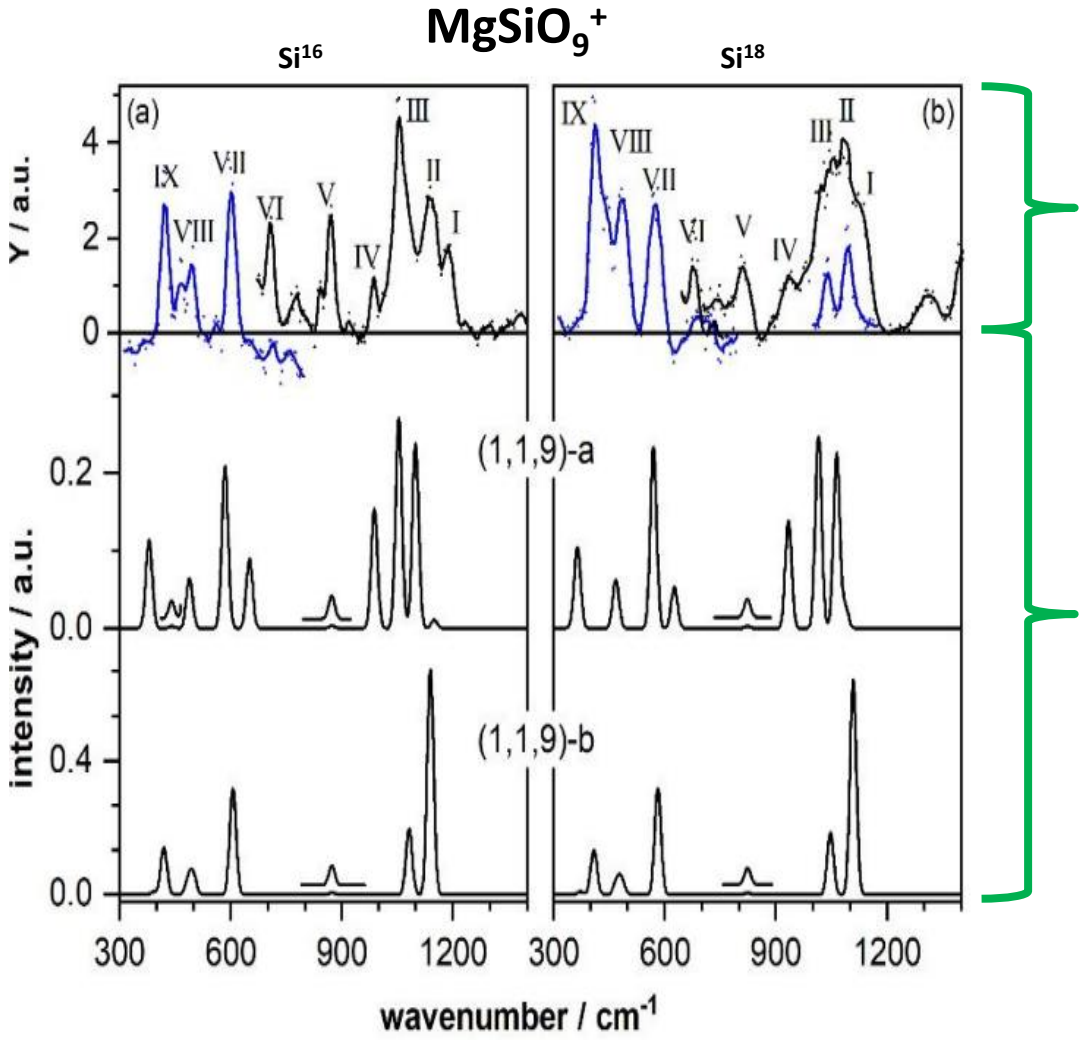

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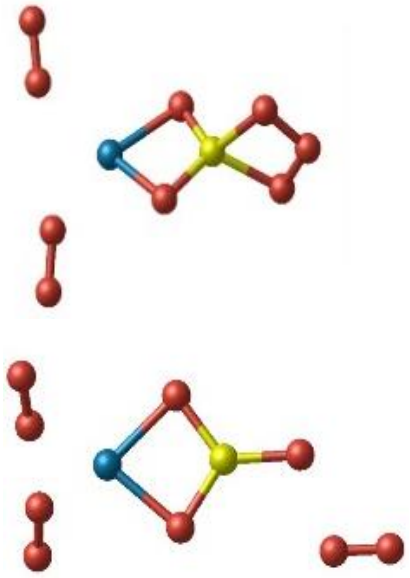
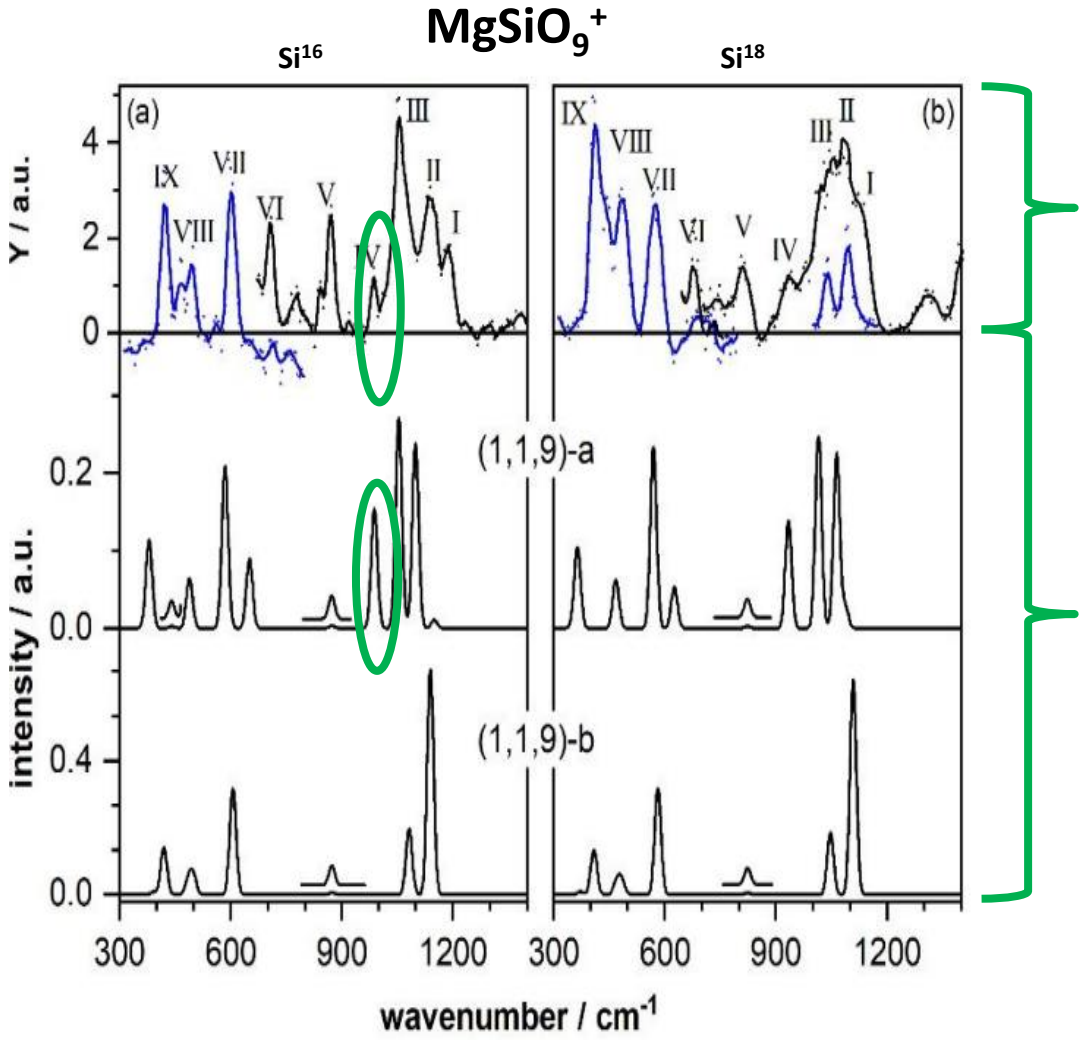
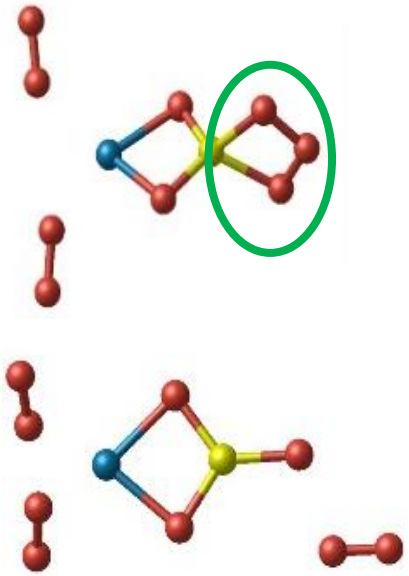


- Good agreement between experiment and models.
- Silicate core responsible for the majority of the signals.

COMPARE IR SPECTRA



EXPERIMENT



- Good agreement between experiment and models.
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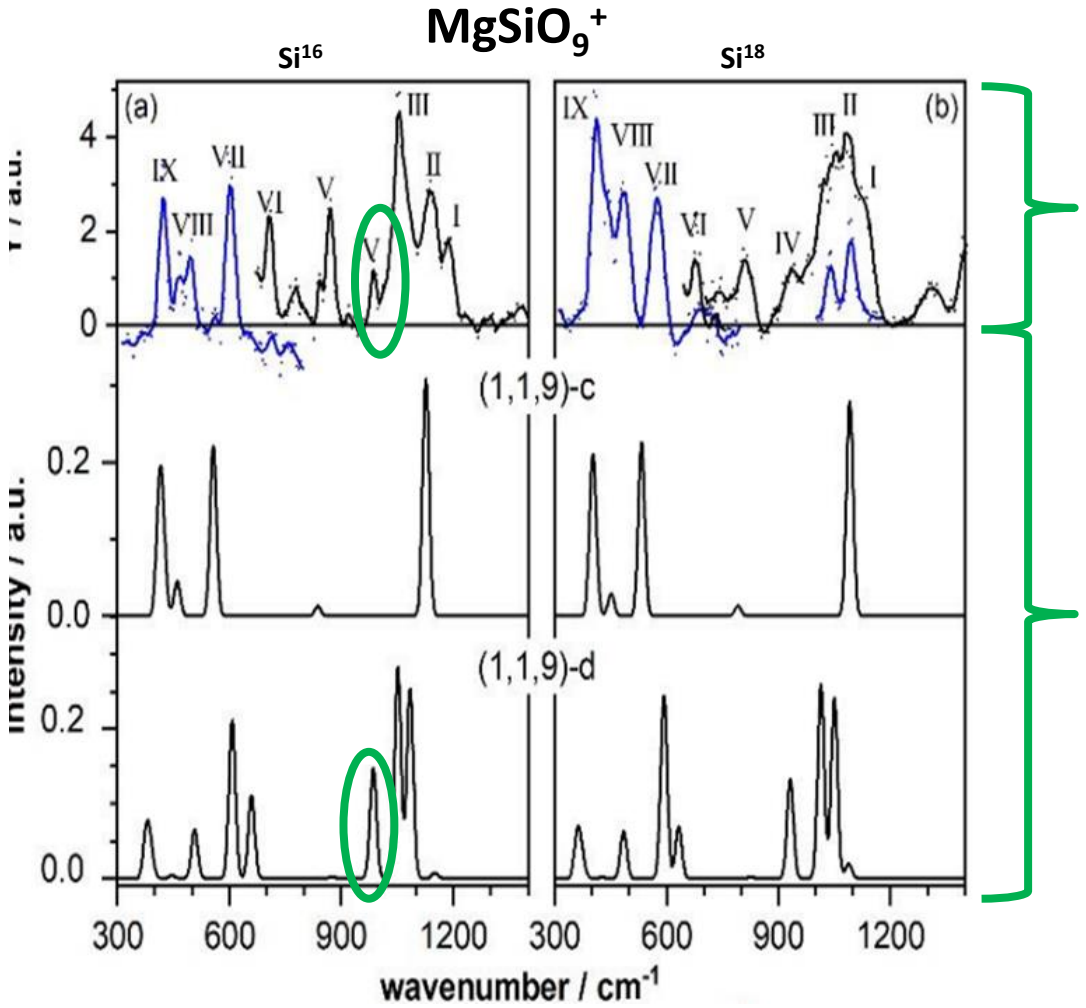
- Ozone-like structure stretching explains experimental band IV

COMPARE IR SPECTRA



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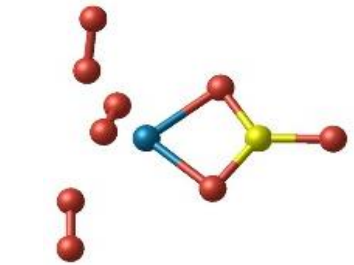

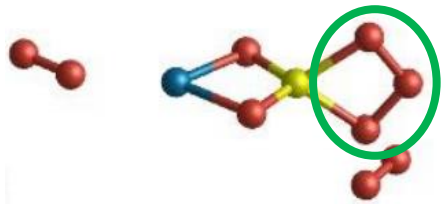

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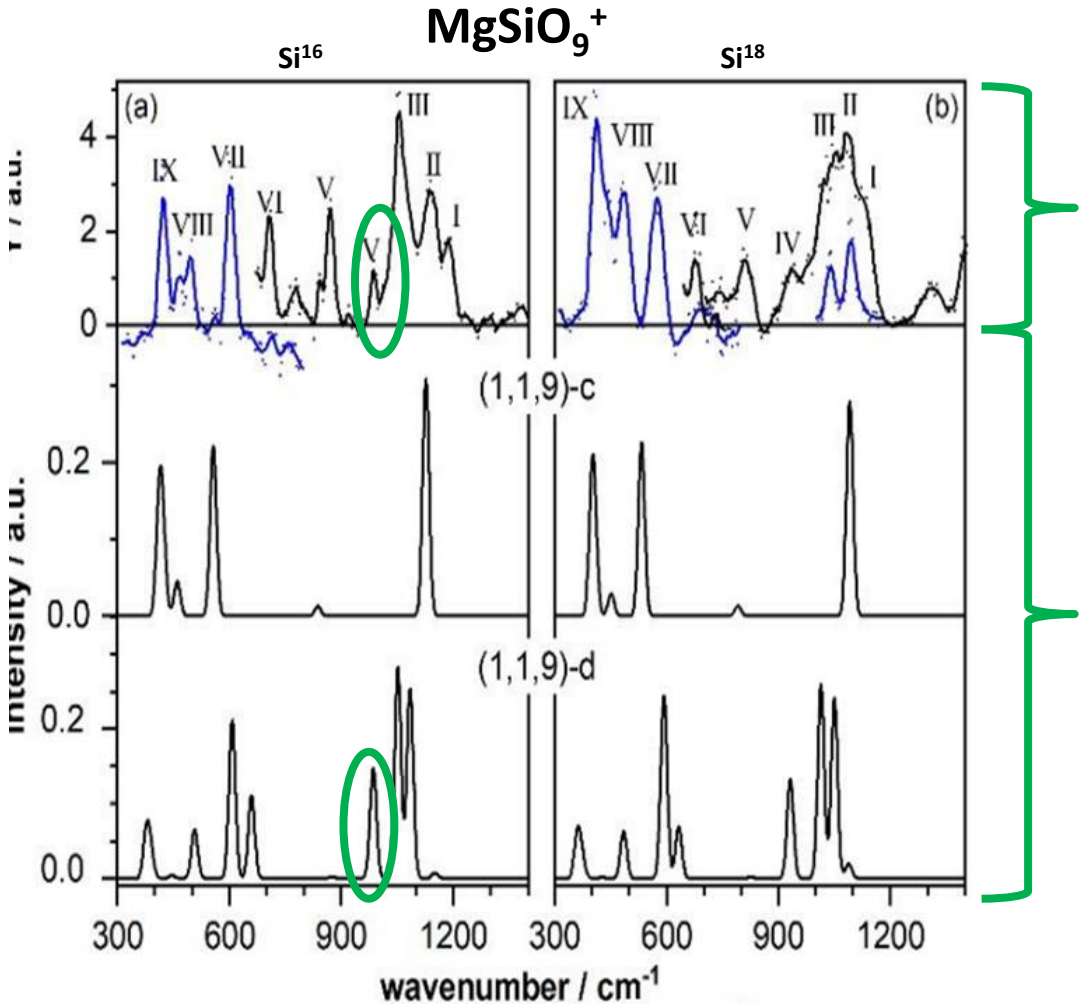

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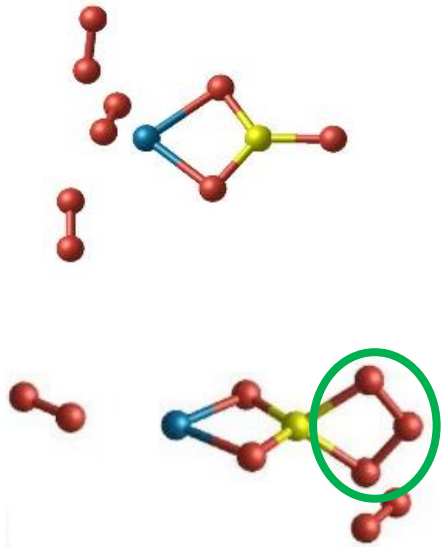

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OUR MODELS ARE GOOD FOR MODELLING IR SPECTRA!

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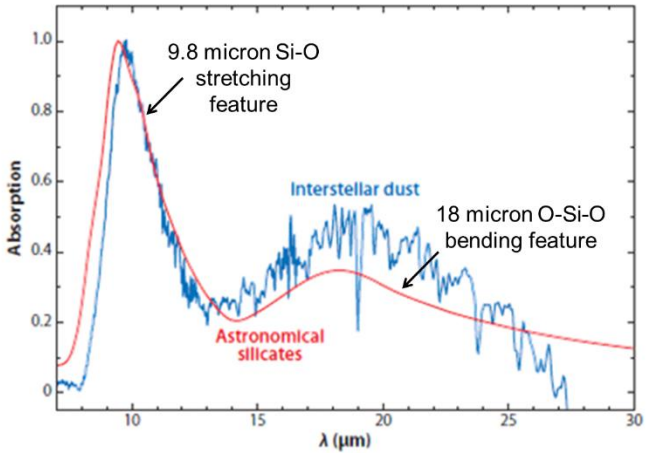
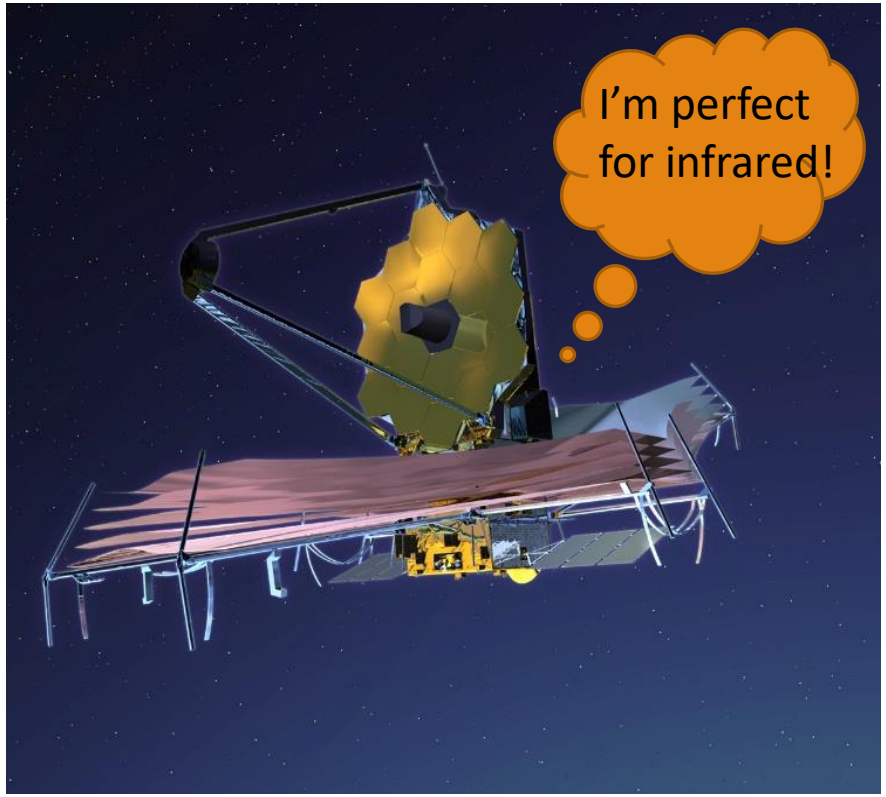


ASTRONOMICAL RELEVANCE

- Models correctly reproduce the IR spectra of nanosilicates.
- Most information about silicates come from the infrared.
- James Webb Space Telescope will allow to confirm nanosilicates presence in space.



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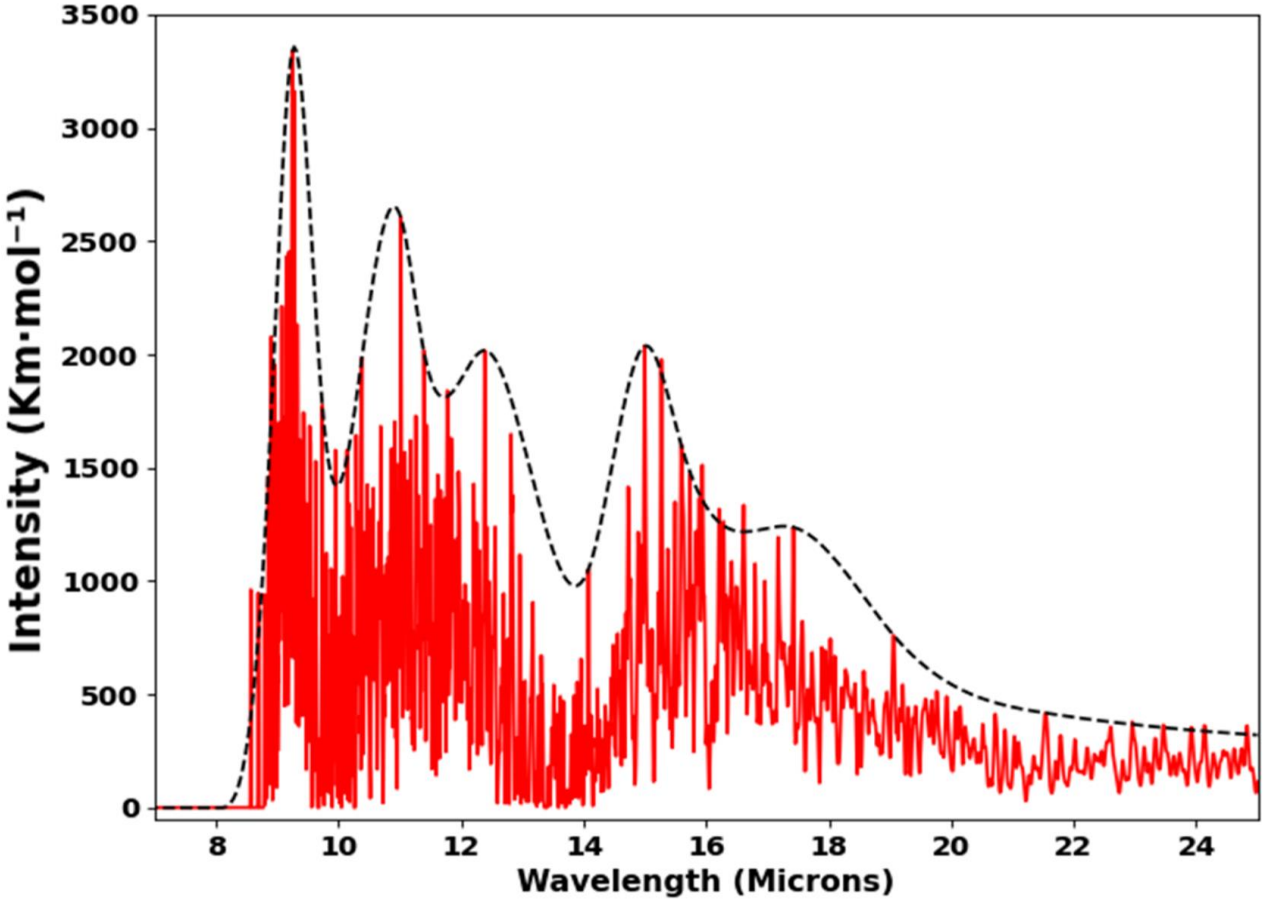

- Nanosilicates population with different size/composition

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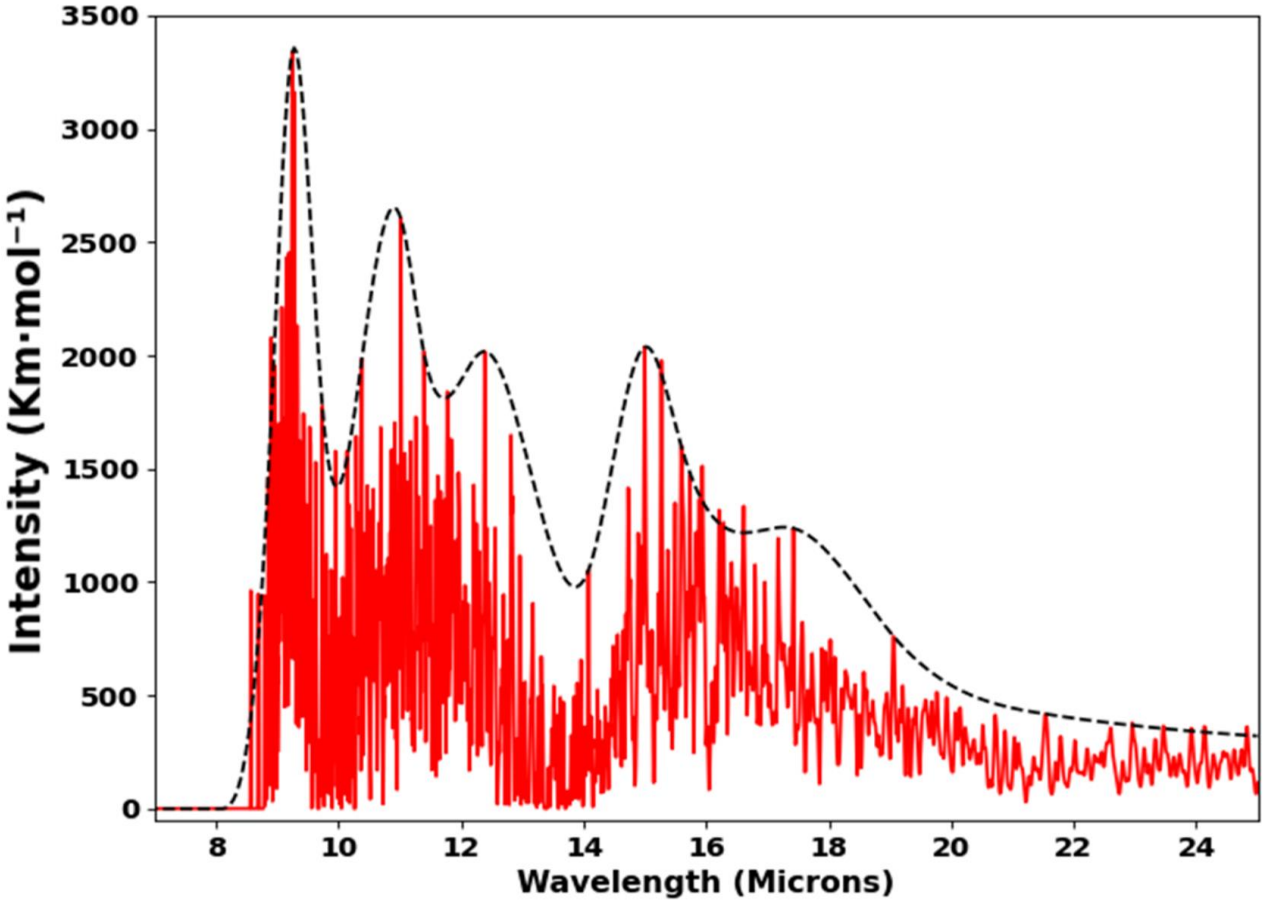

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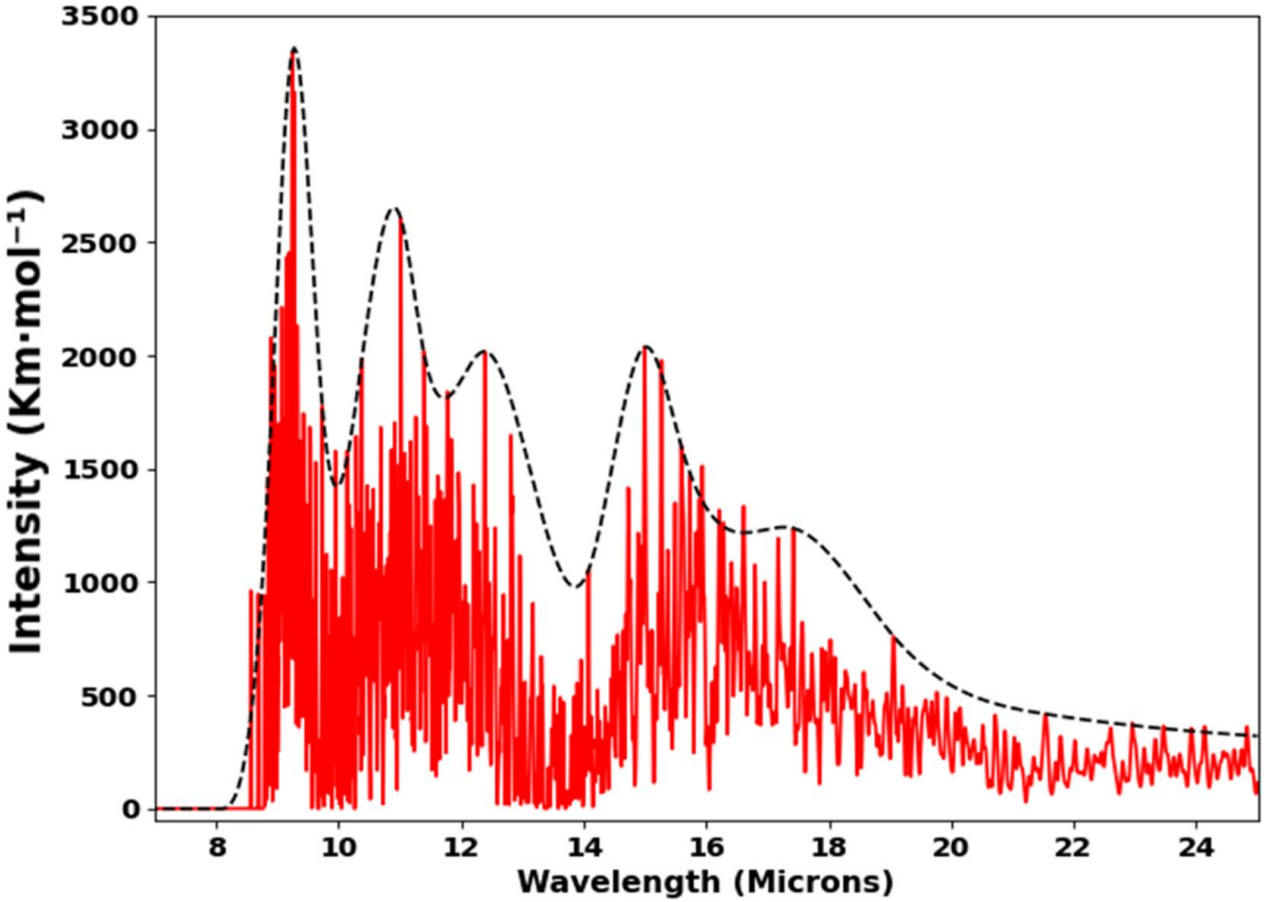

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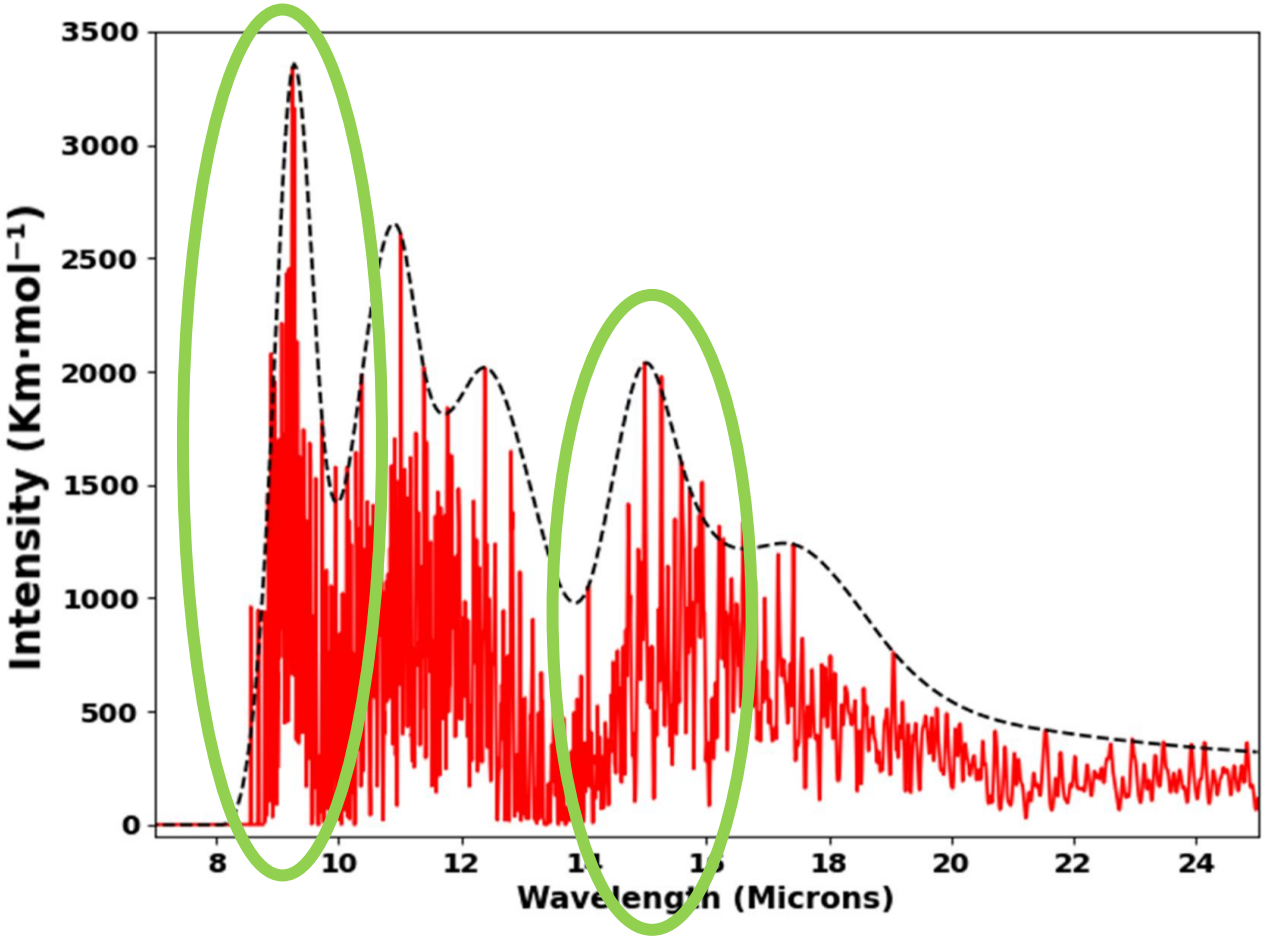
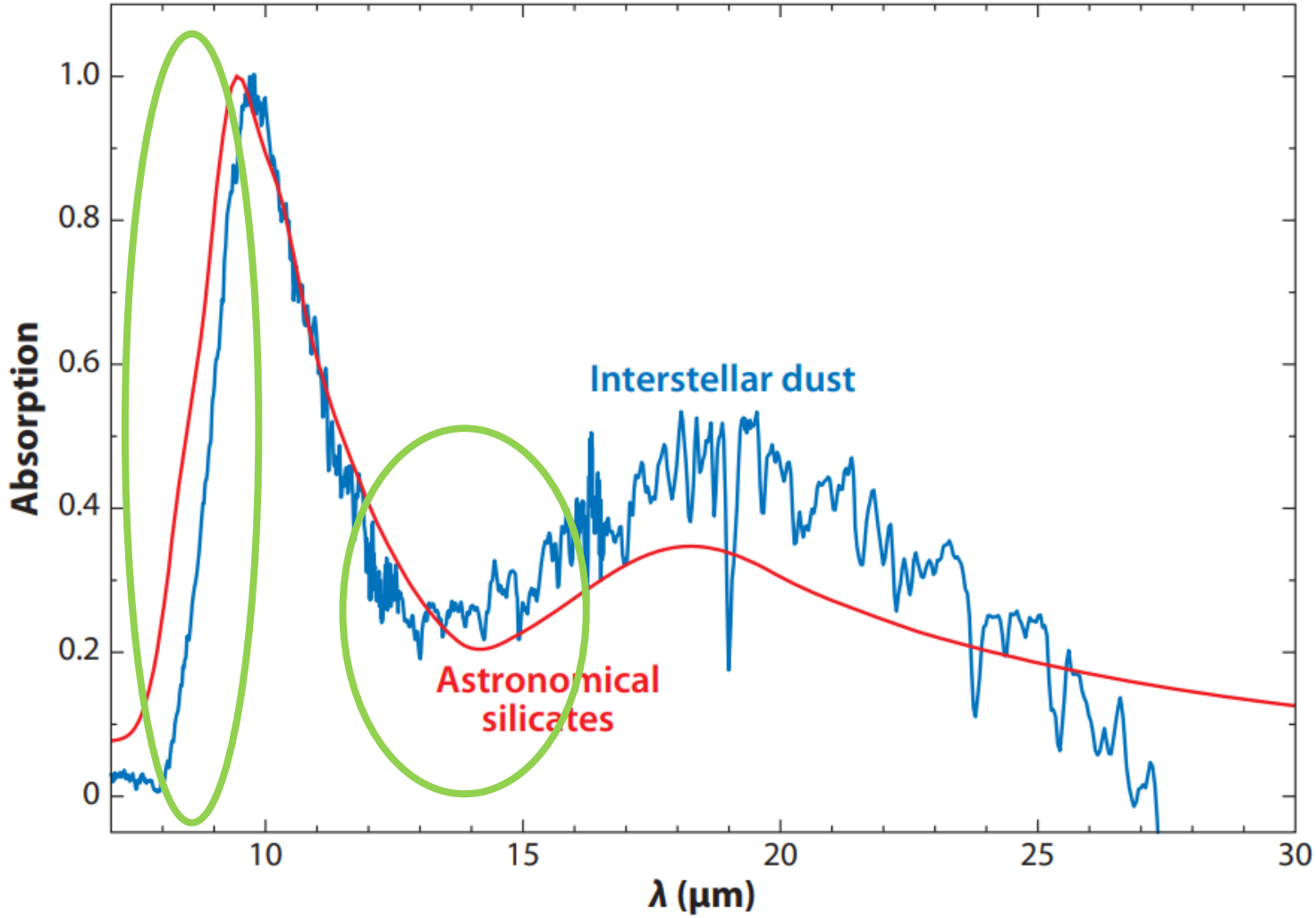


- Nanosilicates population with different size/composition
- Spectrum different than bulk silicates!
- Looks like a shifed version of bulk silicates spectra
- Intensity below 18 and 10 microns

ASTRONOMICAL RELEVANCE



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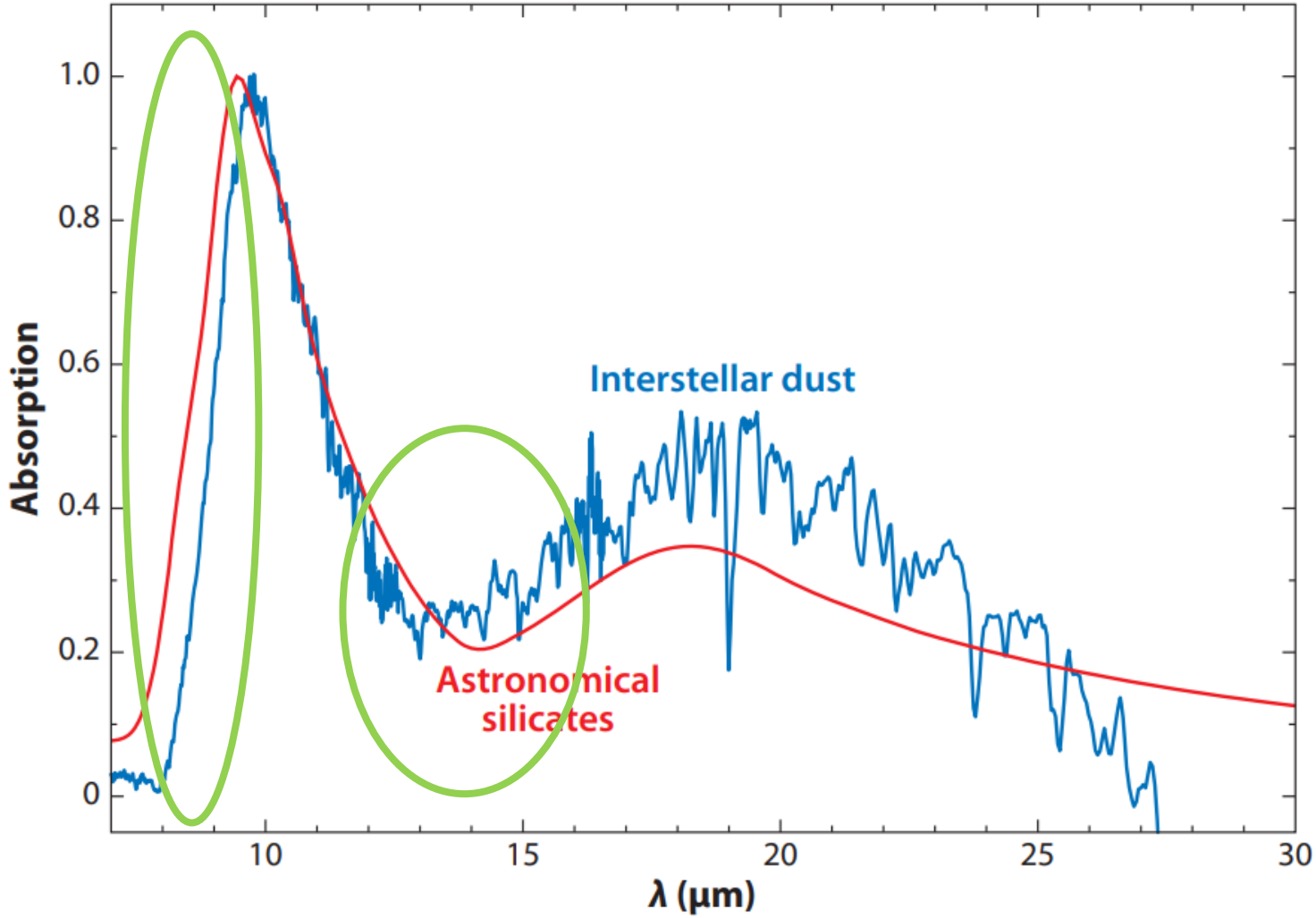
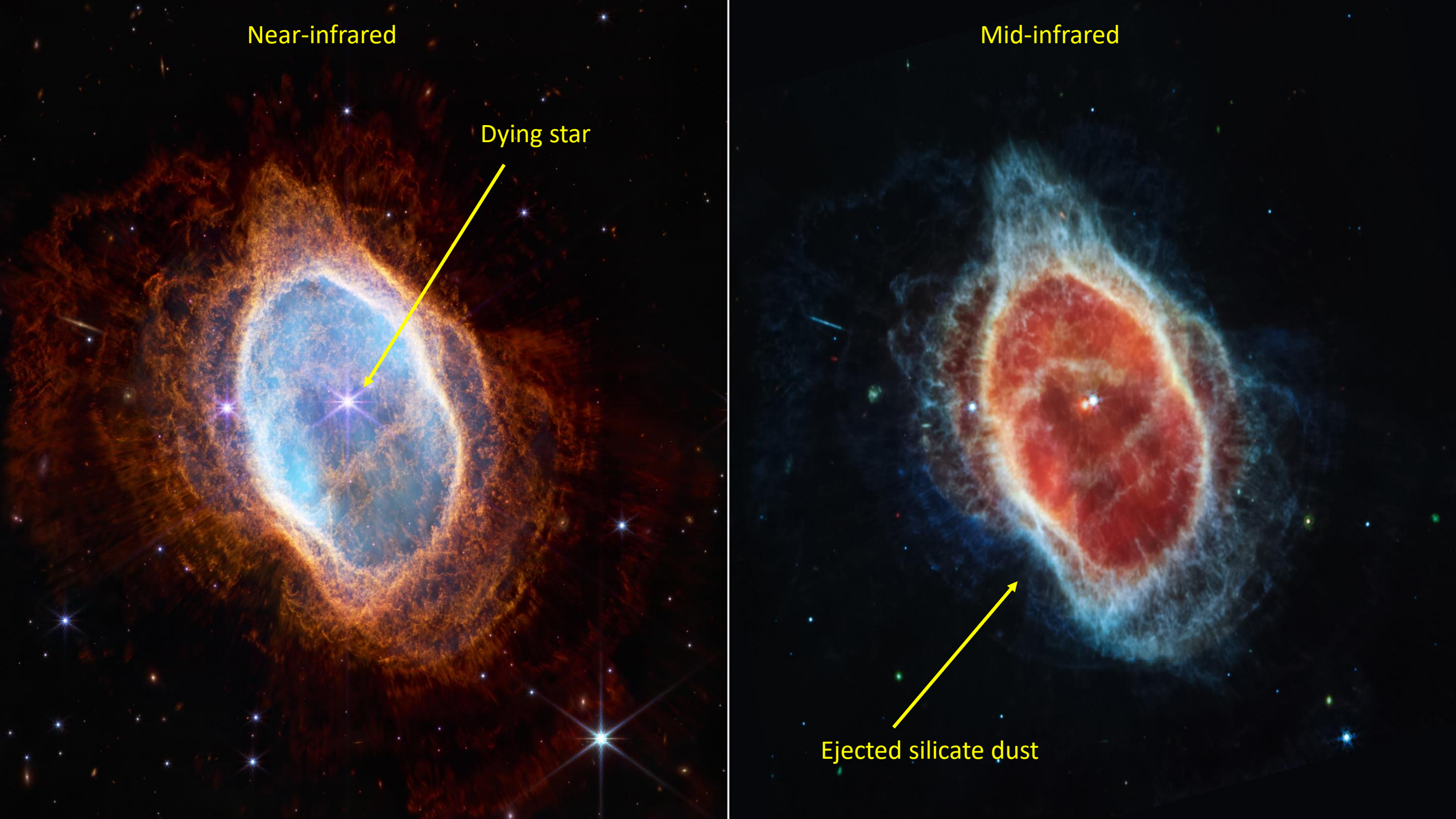


HOPEFULLY, JAMES WEBB WILL SEE FEATURES THERE


Near-infrared
Dying star
Mid-infrared
Ejected silicate dust

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  - **Bianca-Andrea Ghejan**
  - **Dr. Sandra Lang**
  - **Dr. Thorsten Bernhardt**
  - **Dr. Joost Bakker**
- **Webb Investigation of Silicates, Carbons and Ices group**
  - **Dr. Sascha Zeegers**
  - **Prof. Ciska Kemper**
- Supervisor:
  - **Prof. Stefan T. Bromley**

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Institut de Química Teòrica i Computacional
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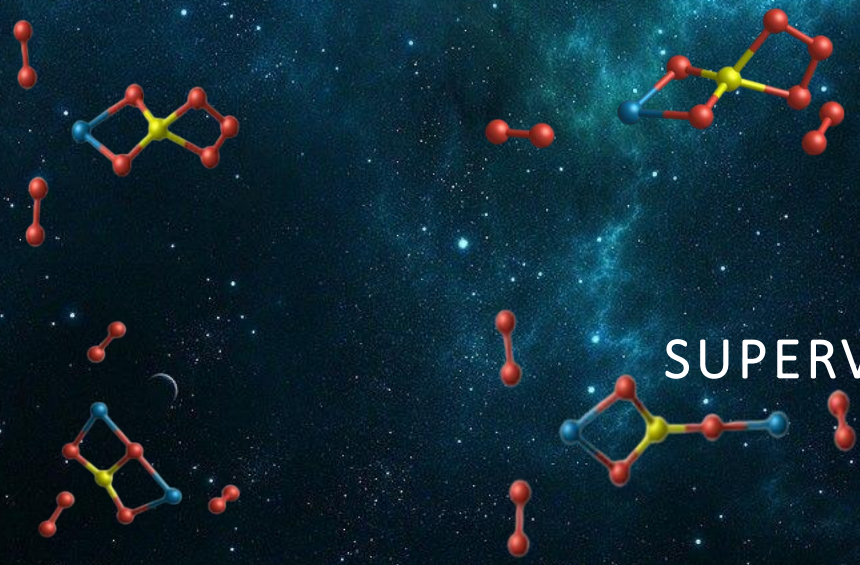
EXCELENCIA MARÍA DE MAEZTU

Nanoclusters & Nanostructured Materials

NANOSILICATE CLUSTERS AND THEIR INTERACTION WITH OXYGEN: ASTRONOMICAL RELEVANCE



JOAN MARIÑOSO GUIU

SUPERVISOR: STEFAN T. BROMLEY

IBER 2023

SEPTEMBER 2023