

## Simulations of CH<sub>4</sub>/H<sub>2</sub>O ices as models for TNOs

R. Escribano,<sup>1</sup> B. Maté,<sup>1</sup> G. Molpeceres,<sup>1</sup> P.C. Gómez,<sup>2</sup> and M.A. Satorre<sup>3</sup>

<sup>1</sup>*Instituto de Estructura de la Materia, IEM-CSIC, Madrid, Spain*

<sup>2</sup>*Departamento de Química-Física I, Universidad Complutense, Unidad Asociada UCM-CSIC, Madrid, Spain*

<sup>3</sup>*Centro de tecnologías Físicas, Universitat Politècnica de València, UPV, Alcoi, Spain*

The arrival of the New Horizons mission to the limits of the solar system has provided new and exciting data on the distant objects found there. Among these data, infrared spectra on a range of locations of the surface of Pluto and Charon have shown the variety of composition of different spots. The spectra reveal the general abundance of CH<sub>4</sub> ice in Pluto, mixed with CO, N<sub>2</sub> and other hydrocarbons, and also the presence of H<sub>2</sub>O at some specific points [1].

The observed spectra cover the near-infrared range, 1.1 to 2.5 μm. Our goal in this work is to make theoretical models for mixtures of ices with various compositions and predict their spectra, aiming to match the New Horizons observations. In a first stage, we are focused on mixtures of CH<sub>4</sub> and H<sub>2</sub>O (see Figure). Previous experimental work of our group in this field consisted in the measurement of optical constants and band strengths of CH<sub>4</sub>/C<sub>2</sub>H<sub>6</sub> in the near- and mid-IR regions [2]. The methodology employed in this work consists in generating amorphous mixtures of the desired composition by means of a molecular dynamics and optimizing their structure searching for the minimum of their potential energy surface. This structure is taken to calculate the harmonic vibrational spectrum, and as a starting point for a molecular dynamics simulation, which will yield also the prediction of the near-IR spectrum. All calculations are carried out by means of Materials Studio software [3], using the Density Functional Theory method, with GGA-PBE functionals and Grimme D2 dispersion correction.

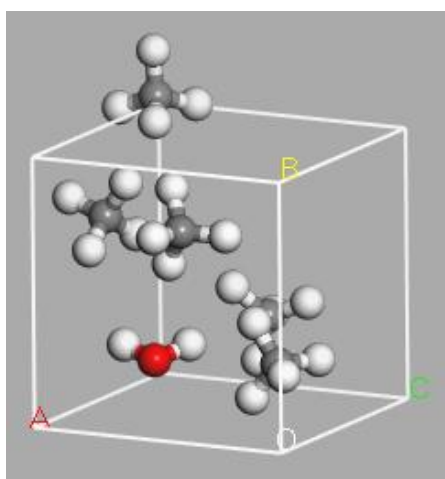


Figure : Relaxed amorphous structure for a 5:1 CH<sub>4</sub>/H<sub>2</sub>O mixture.

### References

- [1] W.M. Grundy et al. *Science*, 351, 1283, 2016.
- [2] G. Molpeceres et al., *Astrophys. J.*, 825:156, 2016.
- [3] S.J. Clark, M.D. Segall, C.J. Pickard, et al., *Z. Krist.* 220, 567, 2005.