Hakima Mokrane, J Astrophys Aerospace Technol 2018, Volume 6
DOI: 10.4172/2329-6542-C7-035

4th International Conference on
ASTROPHYSICS AND PARTICLE PHYSICS
December 03-05, 2018 | Chicago, USA

# Molecular astrophysics: Formation and interaction of molecules and new approach: Deep Learning (AI) in astronomy

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200 different species detected up today in the interstellar and circumstellar media have also been identified in icy environments. The fact that, for most of the species observed so far in the ISM, the most abundant isomer of a given generic chemical formula is the most stable one (MEP) suffers very few exceptions. Two couples of isomers, $CH_3COOH/HCOOCH_3$ and $CH_3CH_2OH/CH_3OCH_3$ whose formation is thought to occur on the icy mantles of interstellar grains. Here, we report a coherent and concerted theoretical/experimental study of the adsorption energies of AA/MF and EtOH/DME on the surface of water ice at low temperature. For each pair of isomers, theory and experiments both agree that it is the most stable isomer (AA or EtOH) that interacts more efficiently with the water ice than the higher energy isomer (MF or DME). This differential adsorption shows clearly in the different desorption temperatures of the isomers. It is not related to their intrinsic stability but linked to the fact that both AA and EtOH make more and stronger hydrogen bonds with the ice surface. The formation of water molecules from the reaction between $O_3$ and D-atoms is studied experimentally for the first time. Ozone is deposited on non-porous amorphous solid water ice and D-atoms are then sent onto the sample held at 10K. HDO molecules are detected during the desorption of the whole substrate where isotope mixing takes place, indicating that water synthesis has occurred. The efficiency of water formation via hydrogenation of ozone is of the same order of magnitude as that found for reactions involving O-atoms or $O_2$ molecules and exhibits no apparent activation barrier. These experiments validate the assumption made by models using ozone as one of the precursors of water formation via solid-state chemistry on interstellar dust grains.

## Biography

Hakima Mokrane is a researcher in laboratory astrophysics and astrochemistry and now a data scientist, she designs algorithms for solving AI problems. She graduated from Orsay university with a master (Joint Honours) Physics and Chemistry, before completing her PhD (in molecular physics and laboratory astrophysics) at Paris observatory and Cergy University. Her interests span "all things ice", looking at how solid state materials play a role in the processes of star and planet-formation. She combines laboratory experiments with major facilities use, to understand the role of ice in interstellar chemistry and planet-forming collisions, and exploit molecular dynamics simulations to understand the physical chemical properties of ice in space. and now she is designing algorithms to solve AI problems and is interested in the problems of machine learning and deep learning.

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