Joan Enrique-Romero

Title:
Surface Computational Astrochemistry on the Formation and Destruction of HCN and HNC – MSCA Postdoctoral Fellowship project “ICE-CN”

Abstract:
HCN and HNC are crucial molecules in the field of astrochemistry. They are routinely used by astronomers to trace temperature and dense gas regions, both within and beyond our galaxy, where stars and planetary systems form. Additionally, they are key precursors of complex species, including prebiotic molecules like amino acids and nucleotides. However, their formation and destruction pathways on interstellar ices remain largely unexplored.
This knowledge gap is the main motivation for my fellowship, which can be divided into two parts. First, I will study the formation and destruction of HCN, HNC, and their deuterated counterparts on water and carbon monoxide interstellar ice models using state-of-the-art computational chemistry and astrochemical modeling. Finally, I will test the generated quantum chemical data by incorporating it into astrochemical models. The modelled abundances will be compared to those derived from astronomical observations in different regions of space.