MINISTERIO
DE CIENCIA
E INNOVACIÓN

CSIC
CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS

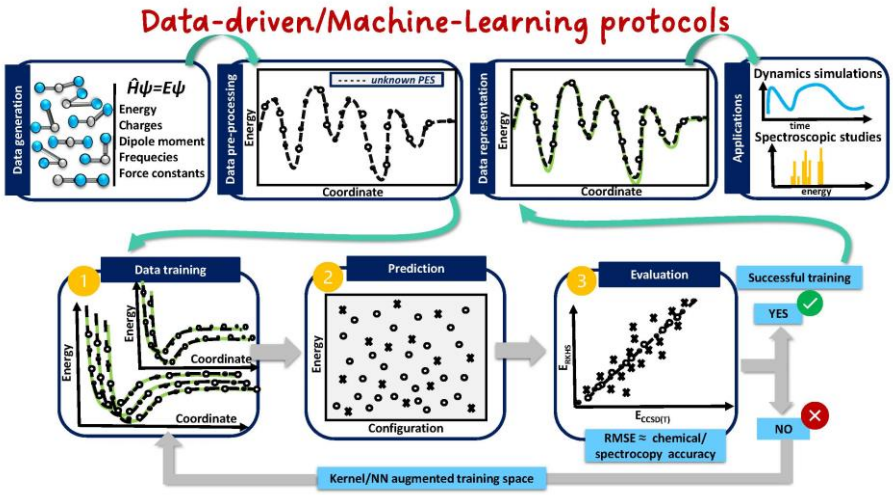
IFF
INSTITUTO DE FÍSICA FUNDAMENTAL

MEMORIA DEL PROGRAMA DE FORMACIÓN

Referencia: **JAEINT23_EX_0190**

Tutor: Dra. Aristea Prosmiti
E-mail: a.prosmiti[at]csic.es

"Challenges in computational characterization of molecular species"



Our research involves investigations at microscopic level using molecular computer simulations, as a powerful tool of a crucial importance if we want a precise understanding of the interaction existing between atoms and molecules or the mechanisms which govern the processes responsible of formation, growth, phase transition or fragmentation of molecular complexes, which otherwise could get hardly accessible through experimentation. The key point for any computational approach to be useful in molecular sciences is the proper modelling of the underlying interactions, to buil up predictive (data-driven via machine learning) models providing detailed knowledge on energetics and structural properties of molecular species under various thermodynamic conditions. Our main goal is to provide response to a series of fundamental questions with relevance in future applications of astrophysical, environmental and energy/storage interest. The training plan includes specific tasks, such as : Bibliography search, Linux operating system, programming in shell script, Python, Fortran, C/C++, high-performance scientific computing, development/implementation of state-of-the-art software (codes and algorithms) in molecular science fields (molecular physics, quantum chemistry, computational modelling, and quantum technologies). The student will also join research activities, such as seminars/workshops/conferences, in collaboration within current international network actions. Our research group participates in the official inter-university "Theoretical Chemistry and Computational Modelling" MSc (Erasmus Mundus) and PhD programs (Faculty of Science, UAM). The student will gain a wide experience in computational molecular and chemical physics, treating with increased complexity molecular systems from gas to condensed phase involving modern (quantum / semiclassical / classical / statistical) methodologies and leading-edge protocols on computational modelling. For more info, please visit: http://fama.iff.csic.es/personas/rita/Publications-RP.html