



Researchers involved	Property
N. Faginas Lago, A. Lombardi)	Dynamics and kinetics of molecular energy transfer in earth and planetary atmospheres
(A. Lombardi, N. Faginas Lago, O. Gervasi)	Classification and recognition of biomolecules by deep learning methods Classification and recognition of biomolecules by deep learning methods
(N. Faginas Lago, A. Lombardi, L. Catacuzzeno)	Protein membrane interaction simulations
(N. Balucani)	Chemistry of the interstellar medium
(N. Balucani)	Chemistry of planetary atmospheres, moons and comets
(N. Balucani)	Combustion chemistry

(F. De Angelis, E. Mosconi, D. Meggiolaro)	Ab initio modeling of metal halide perovskites for photovoltaics and optoelectronics
	Ab initio modeling of dyes, semiconductors and hole transporters for dye-sensitized solar cells (F. De Angelis, S. Fantacci)
(L. Belpassi)	Relativistic DFT: Development and applications
(F. De Angelis, D. Meggiolaro, E. Mosconi)	Computational materials science: Inorganic and organic semiconductors
(P. Belanzoni)	Theoretical inorganic and bioinorganic chemistry
(F. Nunzi)	Optical and electronic properties of molecules in solution and nanomaterials
(S. Fantacci, F. De Angelis)	Modeling electronic and optical properties of transition metal complexes for lighting applications