Gabriele Amante

Data di nascita | **Nazionalità:** Italiana | **Sesso:** Maschile | **Numero di telefono:**

Indirizzo e-mail

Indirizzo

ISTRUZIONE E FORMAZIONE

03/2025 Messina, Italia
LAUREA MAGISTRALE IN PHYSICS Università degli studi di Messina

Livello EQF Livello 7 EQF

07/2021 Messina, Italia
LAUREA TRIENNALE IN FISICA Università degli studi di Messina

Livello EQF Livello 6 EQF

2017 Messina, Italia
DIPLOMA LICEO SCIENTIFICO Scuola Empedocle

COMPETENZE LINGUISTICHE

Lingua madre: **ITALIANO**

Altre lingue:

	COMPRENSIONE		ESPRESSIONE ORALE		SCRITTURA
	Ascolto	Lettura	Produzione orale	Interazione orale	
INGLESE	C1	C1	C1	C1	C1

Livelli: A1 e A2: Livello elementare B1 e B2: Livello intermedio C1 e C2: Livello avanzato

ESPERIENZA LAVORATIVA

2023 – 2024 Messina, Italia
TIROCINIO ISTITUTO PER I PROCESSI CHIMICO-FISICI, CONSIGLIO NAZIONALE DELLE RICERCHE (IPCF-CNR)

Ab initio molecular dynamics simulations of molecular systems.
Development of post processing codes.

2022 Messina, Italia
TUTOR UNIVERSITARIO UNIVERSITÀ DEGLI STUDI DI MESSINA

Tutoring activities on general Physics to Management Engineering bachelor students.

2020 – 2021 Messina, Italia
TIROCINIO ISTITUTO PER I PROCESSI CHIMICO-FISICI, CONSIGLIO NAZIONALE DELLE RICERCHE (IPCF-CNR)

Ab initio molecular dynamics simulations of molecular systems.
Development of post processing codes.

PUBBLICAZIONI

2025

Hydrogen bonding under electric fields: an ab initio molecular dynamics study of liquid hydrogen fluoride

Advancements in computational methods and high-performance computing have significantly enhanced our understanding of molecular systems. Among these, *ab initio molecular dynamics* (AIMD) has proven particularly powerful for exploring the structure and behavior of inter- and intra-molecular interactions. This thesis focuses on hydrogen fluoride (HF) as a model system for investigating hydrogen bonding (H-bonding) under the influence of external electric fields. Unlike water, HF forms simpler but stronger H-bond networks, making it an ideal candidate for studying fundamental H-bond characteristics. A central aim of this work is to establish a robust geometrical criterion for identifying H-bonds in liquid HF, addressing the lack of standardized definitions in such systems. Using AIMD simulations, we analyze the structural and dynamical properties of HF in bulk, both with and without applied static and homogeneous electric fields. The results reveal how electric fields influence molecular dipole orientation, H-bond strength, and molecular dissociation processes. These findings contribute to a deeper understanding of H-bond dynamics and provide insights relevant to fields such as hydrogen-based technologies and the study of electric-field-driven chemical phenomena.

To be submitted

Autori: G.Amante, S. Savasta, F.Saija, G. Cassone

2022

A Computational Quantum-Based Perspective on the Molecular Origins of Life's Building Blocks

The search for the chemical origins of life represents a long-standing and continuously debated enigma. Despite its exceptional complexity, in the last decades the field has experienced a revival, also owing to the exponential growth of the computing power allowing for efficiently simulating the behavior of matter-including its quantum nature-under disparate conditions found, e.g., on the primordial Earth and on Earth-like planetary systems (i.e., exoplanets). In this minireview, we focus on some advanced computational methods capable of efficiently solving the Schro¨dinger equation at different levels of approximation (i.e., density functional theory)-such as ab initio molecular dynamics-and which are capable to realistically simulate the behavior of matter under the action of energy sources available in prebiotic contexts. In addition, recently developed metadynamics methods coupled with first-principles simulations are here reviewed and exploited to answer to old enigmas and to propose novel scenarios in the exponentially growing research field embedding the study of the chemical origins of life.

Autori: G. Amante, J. E. Sponer, J. Sponer, F. Saija, and G. Cassone | **Volume, numero, pagine**: Entropy, 24 (8): 1012.

CONFERENZE E SEMINARI

Reggio Calabria

Cosmos: Il festival della scienza

Organization of informative meetings aimed at high school students, with the aim of introducing computational sciences through concrete and engaging examples. The activity included the preparation of teaching materials, the illustration of real applications (such as numerical simulations and computational models) and direct interaction with students to stimulate curiosity and interest in scientific research

Autorizzo il trattamento dei miei dati personali presenti nel CV ai sensi dell'art. 13 d. lgs. 30 giugno 2003 n. 196 - "Codice in materia di protezione dei dati personali" e dell'art. 13 GDPR 679/16 - "Regolamento europeo sulla protezione dei dati personali".

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