

Dichiarazione candidato commissario

aggiornamento anno 2024

Al Magnifico Rettore
Università degli Studi "Gabriele d'Annunzio"
di Chieti-Pescara

(Barrare quanto di interesse)

- ☐ Procedura proroga biennale per la chiamata di 1 posto di Ricercatore, ai sensi dell'art. 24 della legge 30 dicembre 2010, n. 240 - G.S.D. CHEM-03 (ex S.C. CHIM03) S.S.D. CHEM-03/A (ex S.S.D. CHIM03/B1) presso il Dipartimento di Farmacia (Bando emanato con D.R. 1114 /2021 prot. 65536 del 02/09/2021 ed Avviso pubblicato sulla G.U. n. 75 del 21/09/2021 IV Serie Speciale - Concorsi ed Esami).

Il sottoscritto Lorian Storch nato a CORTONA (AR) il 04/08/1975 residente a CHIETI prov. CH C.A.P. 66100 in via Di Porta Monacisca n° 3 codice fiscale STRLRN75M04D077S docente di II fascia del S.S.D. CHEM-03 G.S.D. CHEM-03/A (ex S.C. CHIM03/B1) presso l'Università degli Studi di "G. d'Annunzio" di Chieti-Pescara dipartimento di Farmacia indirizzo Università Via dei Vestini, 31- 66100 Chieti (CH) docente di II fascia del S.S.D. CHEM-03 G.S.D. CHEM-03/A (ex S.C. CHIM03/B1) presso l'Università degli Studi di "G. d'Annunzio" di Chieti-Pescara dipartimento di Farmacia indirizzo Università Via dei Vestini, 31 - 66100 Chieti (CH) PEC Ateneo di appartenenza ateneo@pec.unich.it

in qualità di membro indicato della Commissione della procedura di cui in oggetto, bandita dall'Università degli Studi "G. d'Annunzio" di Chieti-Pescara,

DICHARA

ai sensi degli artt. 46 e 47 del D.P.R. 28 dicembre 2000, n. 445, e s.m.i., consapevole della responsabilità penale cui poter andare incontro in caso di dichiarazione mendace ed edotto delle sanzioni penali di cui all'art. 76 del D.P.R. sopra citato, ai sensi dell'art. 84 del D.Lgs. n. 163/2006 e s.m.i. di:

- non essere componente dell'organo di direzione politica dell'amministrazione Università "Gabriele d'Annunzio" (Senato Accademico e Consiglio di Amministrazione);
- non ricoprire cariche politiche;
- non essere rappresentante sindacale o designato dalle confederazioni ed organizzazioni sindacali o dalle associazioni professionali;
- non essere stato condannato, anche con sentenza non passata in giudicato, per i reati previsti nel capo I del titolo II del libro secondo del codice penale;
- non aver avuto giudizio negativo ai sensi dell'art. 6, comma 8, della L. 240/2010;
- non essere a conoscenza, al momento dell'assunzione dell'incarico di Commissario della procedura di cui in oggetto, della sussistenza di alcuna situazione che ai sensi dell'art. 51 del codice di procedura civile comporti l'obbligo di astensione dalla partecipazione alla Commissione;
- di non essere attualmente inserito nelle liste dell'ASN degli aspiranti commissari sorteggiabili 2023/2025 ai sensi del D.D. 1211/2023, art. 6, comma 3;
- di non essere stato nominato commissario, nell'anno 2024, in n. 2 procedure attivate dall'Ateneo "G. d'Annunzio";
- di essere in possesso dell'abilitazione Scientifica Nazionale alle funzioni di professore universitario di Prima Fascia nel Settore Concorsuale 03/B1 - FONDAMENTI DELLE SCIENZE CHIMICHE E SISTEMI INORGANICI.
- impegnarsi, qualora in un momento successivo all'assunzione dell'incarico sopraggiunga una delle condizioni di incompatibilità di cui alle vigenti norme, ovvero una situazione (o la conoscenza della sussistenza di una situazione) di conflitto di

interessi, a darne notizia agli altri componenti della Commissione e all'Ateneo e ad astenersi dalla funzione a norma dell'art. 6 bis della L. 241/1990;

- aver preso visione dell'Informativa sul trattamento dei dati personali di cui alla nota prot. 40807/2018 e di essere consapevole che l'Università "G. d'Annunzio" di Chieti-Pescara tratterà i dati contenuti nella presente dichiarazione per gli adempimenti connessi alla presente procedura nel rispetto delle prescrizioni di cui al Regolamento UE n. 679/2016.

Data

Il/la Dichiarante

03/03/2025

Per eventuali comunicazioni relative alla procedura, il/la dichiarante indica i seguenti recapiti:

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INFORMATIVA SUL TRATTAMENTO DEI DATI PERSONALI

Il trattamento dei dati personali avviene in conformità al Regolamento UE 2016/679.

I dati personali sono trattati, anche in via automatizzata, esclusivamente per le finalità di gestione del presente bando e delle procedure ad esso correlate anche in caso di contenzioso.

In ragione di quanto sopra, il commissario è invitato a prendere visione dell'allegato relativo all'informativa sul trattamento dei dati personali (consultabile anche al link: cliccando [QUI](#))

Data

Il/la Dichiarante

03/03/2025

Per la dichiarazione sostitutiva di notorietà, qualora essa non venga sottoscritta in presenza del dipendente addetto, deve essere presentata unitamente a copia fotostatica non autenticata di un documento di identità del sottoscrittore (Art. 38 D.P.R. 445/2000).



Firmato digitalmente da Lorian Storch
Data: 03.03.2025 13:23:38 CET
Organizzazione: UNIVERSITA' DEGLI
STUDI DI CHIETI E
PESCARA/01335970693

Loriano Storchi, PhD

Education

Università degli Studi di Perugia (Italy)

Ph.D. in Chemistry (Computational Chemistry) with a thesis entitled: "Innovative computational strategies for ab-initio Quantum Chemistry: Grid Computing and novel Green's function techniques"

Università degli Studi di Perugia (Italy)

Bachelor Degree in Chemistry (Chemical Physics) with a score of 110/110 cum laude discussing a thesis entitled "Double Molecular Ionization: effects of 'Foreign Imaging' and nuclear dynamics hexa-halide of sulfur"

Qualified as Full Professor in General and Inorganic Chemistry (ASN - MIUR)

Summary

- Over 20 years of experience in programming. Programming languages include, but not limited to, C/C++, Python, Fortran 77/90. Developing both commercial and academic/research software.
- Over 20 years of experience in High Performance Computing, Parallel and Distributed Computing. Working in various fields such as: Machine Learning techniques, Chemoinformatic, Ab-Initio Quantum Chemistry, Computational Chemistry, Computational Physics, High Energy Physics. Experience in Computational Finance
- Over 20 years of Research activity with a multidisciplinary background that is reflected both in the list of my scientific interest, diversify of publications, and as well in my working experience and teaching activity.
- **Languages include:** Italian (mother language), English (advanced), French (basic knowledge)
- **Computer skills include:** Deep knowledge of programming languages: C/C++, Python, Fortran77/90.. Good knowledge of Java, Pascal, Basic, x86 assembly. Deep knowledge of Linux and Unix in general. Excellent knowledge of Microsoft operating systems. Deep knowledge of networks, network protocols and cloud computing. Deep knowledge of computational architecture (such as modern CPU architecture and memory). Deep knowledge of HPC (High-performance computing), including part of the calculation parallel/multithreaded (MPI, Posix Thread, OpenMP, other shared memory techniques and framework like GlobalArray, ScaLAPACK and other HPC libraries and framework), GPGPU platforms (CUDA, OpenCL), and code optimization. Participation in numerous projects in HPC, Parallel Computing, Grid computing, Cloud Computing, managing both the systems engineering, network, and programming. Deep knowledge of Cheminformatics and Machine-Learning (Deep-Learning) techniques

My multidisciplinary background is reflected both in the list of my scientific interests, diversity of my publications and surely in my approach to research. My work activity is mainly devoted to computer simulation in both chemical and physical science. In this way I have acquired wide competences in several programming languages and computational and numerical methods, Machine and Deep Learning techniques, HPC High Performance Computing, parallel and distributed programming, computational architecture (e.g. modern CPU and memory architectures), networks and network protocols.

Soon after my degree in Chemistry (110/110 cum laude), my first work experience was at the Dept. of Chemistry and CNR-ISTM. I have worked mainly as a programmer in various fields mainly focusing on the parallelization of computational chemistry programs with different techniques and paradigms. I worked with the Dept. of Computer Science (Pisa), being involved in many computational projects. In 2003 I started my PhD in Chemistry which I successfully completed in 3 years. During this period, in addition to the research activities, I also worked as a system and network administrator. In 2007 I received a 3-year research grant entitled "Theoretical study of lifetimes of ionized states through Green Functions and non-Hermitian techniques", working also in the field of Relativistic DFT. I also started working as a scientific consultant and programmer with: Molecular Discovery, developing several commercial programs and with CRC (optimization and porting in HPC environments of atmospheric science codes). In 2010 I worked with the INFN for evaluating the computational needs for the Einstein Telescope project, developing codes for gravitational signal analysis. In 2011 I got a 1 year research grant at the ISTM aiming to implement methods for the simulation and characterization of TiO₂ nanostructured materials. I am now Associate Professor at the Univ. of Chieti and I also started working with INFN in Cloud computing and as Software Engineer at CERN working in the L1 Track Finding activity (reconstruction Real-time trace of charged particles using FPGA).

Professional Experience

University G. D'Annunzio
Chieti-Pescara
Associate Professor
June 2020 – present

I am Associate Professor in General and Inorganic Chemistry at the University of Chieti-Pescara, teaching General and Inorganic Chemistry. During this period I worked also as System and Network administrator for the Theoretical Inorganic Chemistry Group, managing network, servers and HPC resources. And collaborating within the local group in the field of Machine and Deep Learning, bio and cheminformatics

University G. D'Annunzio
Chieti-Pescara
Researcher, Assistant Professor
December 2011 – June 2020

I worked as a researcher in General and Inorganic Chemistry at the University of Chieti-Pescara, teaching General and Inorganic Chemistry. During this period, I worked also as System and Network administrator for the Theoretical Inorganic Chemistry Group, managing network, servers and HPC resources. And collaborating within the local group in the field of bio and cheminformatics. In the very last period, I also started a collaboration with a group of Computational Finance mainly involved in the development of High-Performance Computing code related to the evaluation of the Financial Risk.

CNR SCITEC Researcher
January 2017 - present

I am collaborating with the Department of Chemistry of the University of Perugia on projects related to the development of relativistic DFT software. In addition, I am still collaborating as associated researcher also with the ISTM (CNR) acting within the projects related to hybrid and organic photovoltaics (Computational Laboratory for Hybrid and Organic Photovoltaics <http://www.clhyo.org>).

INFN (National Institute of Nuclear Physics)
Researcher
March 2013 – present

I am collaborating with the INFN (National Institute of Nuclear Physics) being involved in the research activity belonging to the CMS experiment. The collaboration is specifically focused in the aspects of computing related to innovative infrastructure solutions based on the CLOUD paradigm, necessary for the deployment of the future computing model. The activity is part of the Working Group "Cloud" INFN Commission for Computing and Networking (local affiliate). During this period I have been involved in **OCP projects**. Member of the BM team that has been granted a Iron Medal at the "**Innovate FPGA2018**" (<http://www.innovatefpga.com>, under the name "**Reconfigurable Computing**") I am currently working on Machine-Learning techniques applied both to the HEP as well as medical data.

CERN (European Organization for Nuclear Research)
Software Engineer
March 2014 – present

I am collaborating as a software engineer at CERN as part of the group CMS (Compact Muon Solenoid) of Perugia. In this contest I am actively engaged in the development and testing of algorithms track fitting. Following the upgrade of the LHC (Large Hadron Collider) in order to prevent the loss of interesting events it will be necessary to use new approaches. In this context the reconstruction Real-time trace of charged articles, may be carried out by the use of Associative Memory and FPGA (Field - Programmable Gate Array). My work is mainly focused on the study and implementation of track fitting algorithms of interest in the project of L1 Track Triggering of the CMS experiment. The study is facing the testing and optimization of the algorithms in order to implement them on a FPGA. As a CERN associated Software Engineer I've been at CERN (Genève) numerous times (Tracker week Phase II upgrade days) to attend meetings and present the results. (Developing a PCA fitter for the L1 track Finding https://github.com/lstorchi/pca_fit and its integration on the CMSSW framework <https://github.com/lstorchi/cmssw>)

Molecular Discovery Ltd., London
UK
Programmer Scientific Consultant
March 2004 - present (**after 2011
present scientific collaboration**)

In this period I worked as a scientific consultant and programmer for Molecular Discovery Ltd., London, UK, participating in the development of many commercial programs, a complete review of which can be found at: <http://www.moldiscovery.com/>. The following list is a subset of the software and scientific contribution that I consider the most significant:

- libgrid/grid: thread safe library and a subsequent (parallel) program inspired by the original GRID developed by Dr. Peter Goodford, a computational procedure for determining energetically favorable binding sites on molecules of known structure. It may be used to study individual molecules such as drugs, molecular arrays such as membranes or crystals, and macromolecules such as proteins, nucleic acids, glycoproteins or polysaccharides. The library is used in several other commercial programs, such as VolSurf+, MetaSite, Almond, Shop, Pentacle, Flap, and more.
- MoKa : in-silico computation of pKa values using a novel approach that provides accurate and fast calculations using an algorithm based on descriptors derived from GRID molecular interaction fields.
- Kibitzer: an automatic and expert tool to expand the MoKa internal database with a corporate database of pKa values.
- libtaut/tauthor: a computational procedure for the enumeration of tautomers and the estimation of their stability in the aqueous medium solution.
- liblogd : a library for logD and logP prediction.
- MoKaBio : in-silico computation of proteins pKa values by environment similarity.
- fixpdb : a procedure for filtering PDB files based also on a PDB residues dictionary.
- DeepGrid: a CBB model to predict various drug-like molecule properties starting from the GRID MIF

(Many of the procedures/libraries mentioned above are used by other commercial programs to which I contributed)

During this period, and this collaboration, I also worked on a number of scientific publications in international journals. Acquisition of competences in using the Qt framework also belongs to this collaboration.

ISTM-CNR (Institute of Molecular
Science and Technologies)
Staff Scientist
June 2011 – December 2011

I have done research activities at the (ISTM (Institute of Molecular Science and Technology) – CNR of Perugia as holder of a research grant aiming to achieve the "Implementation and optimization of non-relativistic and relativistic DFT codes of parallel computer architectures and multi and many cores (GPU)

for advanced simulations materials and processes in organic and hybrid photovoltaics.”. In this period, I improved my skills in Python programming language, and I acquired the skills of VTK (The Visualization Toolkit). The research project involved the development of software and computational techniques for the simulation of TiO₂ nanostructured materials and their characterization, acquiring also skills on computational geometry.

2b Solutions S.R.L.
Programmer Consultant
February 2011 – September 2011

During this period, I worked as a programmer developing a tool for database synchronization in python Joomla! in relation to the project ”Tazebao the XXI century”.

CRC (Center for Research on
Climate and Climate Change)
Programmer Scientific Consultant
May 2011 – December 2011

I worked as a scientific consultant and programmer for the CRC (Center for Research on Climate and Climate Change) in Perugia with object ”Porting and optimization of code meteorological platforms multi and many cores”

INFN (National Institute of Nuclear
Physics)
Staff Scientist
May 2010 – May 2011

I worked as a collaborator with the I.N.F.N. (National Institute of Nuclear Physics) section of Perugia for evaluating the computational needs for the Einstein Telescope project using the Many-Core (GPU) environment. During this period, I developed and optimized codes for gravitational signal analysis, therefore I acquired the basic skills of the DSP (Digital Signal Processing), as well as in the field of Many-Core programming (GPGPU and beyond). Contemporaneously, during this cooperation, I co-wrote the Design Study for the Einstein Telescope. At the same time, I also worked as a consultant for the SCI (Italian Chemical Society) as a staff organizer of the HOPV2010.

Department of Chemistry University
of Perugia
Staff Scientist
January 2007 – December 2009

Grant holder at the University of Perugia entitled ”Theoretical study of lifetimes of ionized states through technical and non-Hermitian Green functions”, with involvement of developing and parallelizing code. In the same period, I carried out activities as a Systems and Network Administrator at the ISTM (Institute of Molecular Sciences and Technologies) and the Department of Chemistry. In the early months of 2009 to carry out activities as a scientific consultant and programmer with The CRC (Center for Research on Climate and Climate Change) of Perugia with object ”Optimizing, porting and management in HPC environments of parallel codes for the simulation of convective weather

phenomena in static equilibrium "played in Project "AMMA - African Monsoon Multidisciplinary Analysis". My research activity starting from this period has been devoted also to Relativistic Density Functional Theory. With a specific focus on simulation of big structures involving heavy and super heavy atoms. Contributing to the implementation, optimization and parallelization of BERTHA (Four-Component Relativistic DFT code).

Department of Chemistry University of Perugia
Ph.D. Student
November 2003 – December 2006

Holder of a PhD scholarship at the Department of Chemistry of the University of Perugia. During this period in addition to the research activities I have worked also at the ISTM (CNR) and the Department Chemistry as a System and Network administrator, managing and configuring network and servers (DNS, mail server, dhcp server, web server, and more) and resources clustered HPC Beowulf. Two of the most significant software contributions of this period are the method not-Dyson ADC (3) (Integral Driven) for the simulation of molecular ionization spectra. As well as a portal based on Java Servlet technology for the simulation of potential energy surfaces on a computing grid. During this time, I also realized the Chemgrid project (in collaboration with several Italian institutions), of which I have studied both the architectural (i.e., sysadmin) and the software aspects.

Department of Computer Science University of Pisa
Research Grant
June 2003 – November 2003

During this period, I worked with the Department of Computer Science University of Pisa for the "Developing Codes ASSIST parallel environment for chemical applications in the strategic project MIUR (High-performance distributed platform)". developing a methodology for dynamic memory allocation within the ASSIST framework.

ISTM (Institute of Molecular Science and Technologies) Department of Chemistry University of Perugia
Research Grant
January 2001 – June 2003

This period belongs to the first practical work experience immediately following my graduation. During these years I have done activities as a programmer in various fields in addition to support skilled in system management and network. I have done research activities having as its object: "Parallelization of computational chemistry programs using Message Passing and Shared Memory techniques", "Development of ASSIST patterns" and "Development of parallel programs (MPI and ASSIST

Programming)". Most of my research activity of this period has been essentially carried out in collaboration with ASI (Italian Space Agency) and the Department of Computer Science (University of Pisa).

Publications list

- Roberto Paciotti, Nazzareno Re, Lorian Storch, "Combining the Fragment Molecular Orbital and GRID Approaches for the Prediction of Ligand-Metalloenzyme Binding Affinity: The Case Study of hCA II Inhibitors", *Molecules*, DOI: 10.3390/molecules29153600 (2024)
- Qizhen Hong, Lorian Storch, Cecilia Coletti, Jia Li, Quanhua Sun, Jun Li, "Quantum-classical rate coefficient datasets of vibrational energy transfer in carbon monoxide based on highly accurate potential energy surface", *The Journal of Chemical Physics*, DOI: 10.1063/5.0189772 (2024)
- Leonardo Arag o, Elisabetta Ronchieri, Giuseppe Ambrosio, Diego Ciangottini, Sara Cutini, Doina Cristina Duma, Pasquale Lubrano, Barbara Martelli, Davide Salomoni, Giusy Sergi, Daniele Spiga, Fabrizio Stracci, Lorian Storch "Air quality changes during the COVID-19 pandemic guided by robust", *Air Quality, Atmosphere and Health*, DOI: 10.1007/s11869-023-01495-x (2024)
- D. Ciangottini, G. Bianchini, M. Mariotti, D. Spiga, L. Storch, G. Surace, "KServe inference extension for an FPGA vendor-free ecosystem", *CHEP2023*, [REF](#) (2023)
- L. Storch within CMS collaboration, "Evaluation of planar silicon pixel sensors with the RD53A readout chip for the Phase-2 Upgrade of the CMS Inner Tracker", *Journal of Instrumentation*, DOI: 10.1088/1748-0221/18/11/P11015 (2023)
- Qizhen Hong, Lorian Storch, Quanhua Sun, Massimiliano Bartolomei, Fernando Pirani, Cecilia Coletti, "Improved Quantum-Classical Treatment of N₂-N₂ Inelastic Collisions: Effect of the Potentials and Complete Rate Coefficient Data Sets", *Journal of Chemical Theory Computation*, DOI: 10.1021/acs.jctc.3c01103 (2023)
- Diego Sorbelli, Paola Belanzoni, Lorian Storch, Olivia Bizzarri, Beatrice Bizzarri, Edoardo Mosconi, Leonardo Belpassi, "Chemical bond analysis for the entire periodic table: energy decomposition and natural orbitals for chemical valence in the four-component relativistic framework", *Molecular Physics*, DOI: 10.1080/00268976.2023.2245061 (2023)
- Lorian Storch, Gabriele Cruciani, Simon Cross, "DeepGRID: Deep Learning using GRID descriptors for BBB prediction", *Journal of Chemical Information and Modeling*, DOI: 10.1021/acs.jcim.3c00768 (2023)
- Tommaso Tedeschi, Marco Baiocchi, Diego Ciangottini, Valentina Poggioni, Daniele Spiga, Lorian Storch, Mirco Tracolli, "Smart Caching in a Data Lake for High Energy Physics Analysis", *Journal of Grid Computing*, DOI: 10.1007/s10723-023-09664-z (2023)
- Qizhen Hong, Lorian Storch, Massimiliano Bartolomei, Fernando Pirani, Quanhua Sun, Cecilia Coletti, "Inelastic N₂+H₂ collisions and quantum-classical rate coefficients: large datasets and machine learning predictions" *The European Physical Journal D*, DOI: 10.1140/epjd/s10053-023-00688-4 (2023)
- Tommaso Tedeschi, Marco Baiocchi, Diego Ciangottini, Valentina Poggioni, Daniele Spiga, Lorian Storch, Mirco Tracolli, "Smart Caching in a Data Lake for High Energy Physics Analysis", *Journal of Grid Computing*, DOI: (2023)

- L. Storchi within CMS collaboration, "Beam test performance of a prototype module with Short Strip ASICs for the CMS HL-LHC tracker upgrade", DOI: 10.1088/1748-0221/17/06/P06039 (2022)
- Daniele Spiga, Diego Ciangottini, Alessandro Costantini, Sara Cutini, Cristina Duma, Jacopo Gasparetto, Pasquale Lubrano, Barbara Martelli, Elisabetta Ronchieri, Davide Salomoni, Giusy Sergi, Lorian Storchi, Mirco Tracoli, "Open-source and cloud-native solutions for managing and analyzing heterogeneous and sensitive clinical Data", *Proocing of Science*, <https://pos.sissa.it/415/022/pdf> (2022)
- Udaykumar Gajera, Lorian Storchi, Danila Amoroso, Francesco Delodovici, Silvia Picozzi "Towards machine learning for microscopic mechanisms:a formula search for crystal structure stability based on atomic properties" *Journal of Applied Physics* DOI: 10.1063/5.0088177 (2022)
- Guglielmo D'Amico , Stefania Scocchera , Lorian Storchi, "Randentropy: A Software to Measure Inequality in Random Systems", *INFORMATICA* DOI: 10.15388/22-INFOR479 (2022)
- L. Storchi within CMS collaboration, "Comparative evaluation of analogue front-end designs for the CMS Inner Tracker at the High Luminosity LHC", *Journal of Instrumentation*, DOI: 10.1088/1748-0221/16/12/P12014 (2021)
- Mirko Mariotti, Daniel Magalotti, Daniele Spiga, Lorian Storchi, "The BondMachine, a moldable computer architecture", *Parallel Computing* DOI: 10.1016/j.parco.2021.102873 (2021)
- Tommaso Tedeschi, Mirco Tracoli, Diego Ciangottini, Daniele Spiga, Lorian Storchi, Marco Baioletti, Valentina Poggioni, "Reinforcement Learning for Smart Caching at the CMS experiment", *PoS(ISGC2021)009*, DOI: 10.22323/1.378.0009 (2021)
- L. Storchi within CMS collaboration, "Selection of the silicon sensor thickness for the Phase-2", *Journal of Instrumentation*, DOI: 10.1088/1748-0221/16/11/P11028 (2021)
- Sara Tortorella, Emanuele Carosati, Giovanni Bocci, Simon Cross, Gabriele Cruciani, Lorian Storchi, Cover Image, *Journal of Computational Chemistry*, DOI: 10.1002/jcc.26756 (2021)
- Sara Tortorella, Emanuele Carosati, Giovanni Bocci, Simon Cross, Gabriele Cruciani, Lorian Storchi, "Combining Machine Learning and Quantum Mechanics Yields More Chemically-Aware Molecular Descriptors for Medicinal Chemistry Applications", *Journal of Computational Chemistry*, DOI: 10.1002/jcc.26737 (2021) - **Top downloaded article (Wiley)**
- Iogann Tolbatov, Tiziano Marzo, Cecilia Coletti, Diego La Mendolace, Lorian Storchi, Nazzareno Re, Alessandro Marrone, "Reactivity of antitumor coinage metal-based N-heterocyclic carbene complexes with cysteine and selenocysteine protein sites", *Journal of Inorganic Biochemistry*, DOI: 10.1016/j.jinorgbio.2021.111533 (2021)
- Mariangela Agamennone, Lorian Storchi, Alessandro Marrone, Roberto Paciotti, "Hampering the early aggregation of PrP-E200K protein by charge-based inhibitors: a computational study", *Journal of Computer-Aided Molecular Design*, DOI: 10.1007/s10822-021-00393-7 (2021)
- L. Storchi within the CMS Collaboration, "The CMS Phase-1 pixel detector upgrade", *Journal of Instrumentation*, DOI: 10.1088/1748-0221/16/02/p02027 (2021).
- Gianpiero Marconi, Domenico Aiello, Bryan Kindiger, Lorian Storchi, Alessandro Marrone, Lara Reale, Niccolò Terzaroli, Emidio Albertini, "The Role of APOSTART in Switching between Sexuality and Apomixis in *Poa pratensis*", *Genes*, DOI: 10.3390/genes11080941 (2020).
- Matteo De Santis, Leonardo Belpassi, Christoph R. Jacob, André Severo Pereira Gomes, Francesco Tarantelli, Lucas Visscher, and Lorian Storchi, "Environmental effects with Frozen Density Embedding in Real-Time Time-Dependent Density Functional Theory using localized basis functions", *Journal of Chemical Theory and Computation*, DOI: 10.1021/acs.jctc.0c00603 (2020).
- Leonardo Belpassi, Matteo De Santis, Harry M. Quiney, Francesco Tarantelli, Lorian Storchi, "BERTHA: Implementation of a four-component Dirac-Kohn-Sham relativistic framework", *The Journal of Chemical Physics*, DOI: 10.1063/5.0002831 (2020).

- L. Storch within the CMS Collaboration, "Experimental study of different silicon sensor options for the upgrade of the CMS Outer Tracker", Journal of Instrumentation, DOI: 10.1088/1748-0221/15/04/P04017 (2020).
- L. Storch within the CMS Collaboration, "Beam test performance of prototype silicon detectors for the Outer Tracker for the Phase-2 Upgrade of CMS", JOURNAL OF INSTRUMENTATION, DOI: 10.1088/1748-0221/15/03/P03014 (2020).
- Roberto Paciotti, Mariangela Agamennone, Cecilia Coletti, Lorian Storch, "Characterization of PD&L1 binding sites by a combined FMO/GRID&DRY approach", Journal of Computer-Aided Molecular Design, DOI: 10.1007/s10822-020-00306-0 (2020).
- Elisa Rossi, Matteo De Santis, Diego Sorbelli, Lorian Storch, Leonardo Belpassi, Paola Belanzoni, "Spin-orbit coupling is the key to unraveling intriguing features of the halogen bond involving astatine", Physical Chemistry Chemical Physics, DOI: 10.1039/C9CP06293A (2020). - **Selected as a 2020 HOT Article**
- M. De Santis, L. Storch, L. Belpassi, H. M. Quiney, F. Tarantelli, "PyBERTHART: A Relativistic Real-Time Four-Component TDDFT Implementation Using Prototyping Techniques Based on Python", Journal of Chemical Theory and Computation, DOI: 10.1021/acs.jctc.0c00053 (2020).
- Guglielmo D'Amico, Stefania Scocchera and Lorian Storch, "On the Sensitivity of a Dynamic Measure of Financial Inequality", Journal of Mathematics and Statistics, DOI: 10.3844/jmssp.2019.280.297 (2019).
- Roberto Paciotti, Iogann Tolbatov, Alessandro Marrone, Lorian Storch, Nazzareno Re, Cecilia Coletti, "Computational chemistry approaches in the study of bioinorganic systems: the case of calcium, gold and platinum ions" ICCMSE 2019 PROCEEDINGS - AIP CP Volume 2186 are now published online, DOI: 10.1063/1.5137922 (2019)
- Lorian Storch, Matteo De Santis, Leonardo Belpassi, "BERTHA and PyBERTHA: State of the Art for Full Four-Component Dirac-Kohn-Sham Calculations", Advances in Parallel Computing, Parallel Computing: Technology Trends, DOI: 10.3233/APC200060 (2019)
- Guglielmo D'Amico, Stefania Scocchera and Lorian Storch, "On the Sensitivity of a Dynamic Measure of Financial Inequality", Journal of Mathematics and Statistics, DOI: 10.3844/jmssp.2019.280.297 (2019).
- Guglielmo D'Amico, Filippo Petroni, Philippe Regnault, Stefania Scocchera, Lorian Storch, "A copula based Markov Reward approach to the credit spread in European Union", Journal: Applied Mathematical Finance, DOI: 10.1080/1350486X.2019.1702068 (2019).
- Mirko Mariotti, Lorian Storch, Daniele Spiga, Davide Salomoni, Tommaso Boccali, Daniele Bonaccorsi, "The BondMachine toolkit: Enabling Machine Learning on FPGA", PoS Proceedings of Science DOI: 10.22323/1.351.0020 (2019).
- L. Storch within CMS Collaboration, "The DAQ and control system for the CMS Phase-1 pixel detector upgrade", Journal of Instrumentation, DOI: 10.1088/1748-0221/14/10/P10017 (2019).
- Guglielmo D'Amico, Stefania Scocchera and Lorian Storch, "On the Sensitivity of a Dynamic Measure of Financial Inequality", Journal of Mathematics and Statistics, DOI: 10.3844/jmssp.2019.280.297 (2019).
- Matteo De Santis, Sergio Rampino, Lorian Storch, Leonardo Belpassi, Francesco Tarantelli, "The Chemical Bond and s-d Hybridization in Coinage Metal(I) Cyanides", Inorganic Chemistry, DOI: 10.1021/acs.inorgchem.9b01694 (2019).
- Carla Maria Coppola, Iogann Tolbatov, Ionut Claudiu Tranca, Cecilia Coletti, Alessandro Marrone, Lorian Storch, Pietro Di Profio, Nazzareno Re, Mher V. Kazandjian, Antonello Pellicchia, Savino Longo, Silvia Gaastra-Nedea, "A database approach for materials selection for hydrogen storage in

- aerospace technology", *Rendiconti Lincei. Scienze Fisiche e Naturali*, DOI: 10.1007/s12210-019-00805-9 (2019).
- Lorian Storchi, Anna Lisa Remoli, Giulia Marsili, Chiara Acchioni, Marta Acchioni, Angela Battistini, Marco Sgarbanti Alessandro Marrone, "A model of the three-dimensional structure of human interferon responsive factor 1 and its modifications upon phosphorylation or phosphorylation-mimicking mutations", *Journal of Biomolecular Structure and Dynamics*, DOI: 10.1080/07391102.2018.1557558 (2019).
 - R. Paciotti, L. Storchi, A. Marrone, "An insight of early PrP-E200K aggregation by combined molecular dynamics/fragment molecular orbital approaches", *Proteins: Structure, Function and Bioinformatics* DOI: 10.1002/prot.25621 (2019).
 - L. Storchi within the CMS Collaboration, "Precision measurement of the structure of the CMS inner tracking system using nuclear interactions", *Journal of Instrumentation*, DOI: 10.1088/1748-0221/13/10/P10034 (2018).
 - M. Mariotti, L. Storchi, D. Spiga, G. Vitillaro, M. Traccolli, D. Ciangottini, M. Ciangottini, V. Formato, M. Duranti, M. Merge', P. D'Angeli, R. Primavera, A. Guerra, L. Fano' and B. Bertucci, "Harvesting dispersed computational resources with Openstack: a Cloud infrastructure for the Computational Science community", *Proceedings of science*, DOI: 10.22323/1.327.0009 (2018).
 - Guglielmo D'Amico, Philippe Regnault, Stefania Scocchera, and Lorian Storchi, "A Continuous-Time Inequality Measure Applied to Financial Risk: The Case of the European Union", *International Journal of Financial Studies*, DOI: 10.3390/ijfs6030062 (2018).
 - D. Rongai, N. Sabatini, P. Pulcini, C. Di Marco, L. Storchi, A. Marrone, "Effect of pomegranate peel extract on shelf life of strawberries: computational chemistry approaches to assess antifungal mechanisms involved", *Journal of Food Science and Technology*, DOI: 10.1007/s13197-018-3192-0 (2018).
 - D'Amico G., Scocchera S., Storchi L., "Financial risk distribution in European Union", *Physica A: Statistical Mechanics and its Applications*, DOI: 10.1016/j.physa.2018.03.069 (2018).
 - De Santis M., Belapassi L., Tarantelli F., Storchi L., "Relativistic quantum chemistry involving heavy atoms", *Rendiconti Lincei. Scienze Fisiche e Naturali*, DOI: 10.1007/s12210-018-0706-7 (2018).
 - L. Storchi within the CMS Collaboration, "Test beam demonstration of silicon microstrip modules with transverse momentum discrimination for the future CMS tracking detector", *Journal of Instrumentation*, DOI: 10.1088/1748-0221/13/03/P03003 (2017).
 - De Santis M., Rampino S., Quiney H.M., Belpassi L., Storchi L. "Charge-displacement analysis via natural orbitals for chemical valence in the four-component relativistic framework", *Journal of Chemical Theory and Computation*, DOI: 10.1021/acs.jctc.7b01077 (2018).
 - Guido Magazzu, Christos Gentsos, Geoffrey Christian Galbit, Gian Mario Bilei, Giacomo Fedi, Lorian Storchi, Daniel Magalotti, Oliver Sander, Atanu Modak, Denis Tcherniakhovski, Fabrizio Palla, Bruno Checcucci, Suvankar Roy Chowdhury, Guillaume Baulieu, Sebastien Viret, Matthias Norbert Balzer, "A real-time demonstrator for track reconstruction in the CMS L1 Track-Trigger system based on custom Associative Memories and high-performance FPGAs", *PoS: Proceedings of Science optical Workshop on Electronics for Particle Physics*, DOI: 10.22323/1.313.0138 (2017).
 - L. Storchi within the CMS Collaboration [2017], "Characterisation of irradiated thin silicon sensors for the CMS phase II pixel upgrade", *European Physical Journal C*, DOI: 10.1140/epjc/s10052-017-5115-z (2017).
 - L. Storchi within the CMS Collaboration, "P-Type Silicon Strip Sensors for the new CMS Tracker at HL-LHC", *Journal of Instrumentation*, DOI: 10.1088/1748-0221/12/06/P06018 (2017).

- Gentsos, C; Fedi, G; Magazzu, G; Magalotti, D; Modak, A; Storchi, L; Palla, F; Bilei, GM; Biesuz, N; Chowdhury, SR; Crescioli, F; Checcucci, B; Tcherniakhovski, D; Galbit, GC; Baulieu, G; Balzer, MN; Sander, O; Viret, S; Servoli, L; Nikolaidis, S, "Track Finding Mezzanine for Level-1 Triggering in HL-LHC Experiments", 2017 6th International Conference on Modern Circuits and Systems Technologies, MOCAS DOI: 10.1109/MOCAS.2017.7937676 (2017).
- L. Storchi within the CMS Collaboration [2017] , "Test beam performance measurements for the Phase I upgrade of the CMS pixel detector", Journal of Instrumentation, DOI: 10.1088/1748-0221/12/05/P05022 (2017).
- L. Storchi within the CMS Collaboration [2017] "Mechanical stability of the CMS strip tracker measured with a laser alignment system", Journal of Instrumentation, DOI: 10.1088/1748-0221/12/04/P04023 (2017).
- S. Rampino, L. Storchi, A. Lagana', "Automated Simulation of Gas-Phase Reactions on Distributed and Cloud Computing Infrastructures", Lecture Notes in Computer Science, DOI: 10.1007/978-3-319-62398-6_5 (2017).
- A. Marrone, N. Re, L. Storchi, "The Effects of Ca²⁺ Concentration and E200K Mutation on the Aggregation Propensity of PrPC: A Computational Study", PloS ONE, DOI: 10.1371/journal.pone.0168039 (2016).
- L. Alunni, N. Biesuz, G.M. Bilei, S. Citraro, F. Crescioli, L. Fano', G. Fedi, D. Magalotti, G. Magazzu¹, L. Servoli, L. Storchi, F. Palla, P. Placidi, A. Papi, Y. Piadyk, E. Rossi, A. Spiezia, "A pattern recognition mezzanine based on associative memory and FPGA technology for L1 track triggering at HL-LHC", Nuclear Instruments and Methods in Physics Research A, DOI: 10.1016/j.nima.2015.09.086 (2015),
- L. Storchi within the CMS Collaboration [2016]: "Trapping in proton irradiated p(+)-n-n(+) silicon sensors at fluences anticipated at the HL-LHC outer tracker", JOURNAL OF INSTRUMENTATION, DOI: 10.1088/1748-0221/11/04/P04023 (2016).
- D. Magalotti, L. Alunni, N. Biesuz, G.M. Bilei, S. Citraro, F. Crescioli, L. Fano', G. Fedi, G. Magazzu, L. Servoli, L. Storchi, F. Palla, P. Placidi, E. Rossi, A. Spiezia, "A Pattern Recognition Mezzanine based on Associative Memory and FPGA technology for Level 1 Track Triggers for the HL-LHC upgrade", Journal of Instrumentation (JINST), Topical Workshop on Electronics for Particle Physics, DOI: 10.1088/1748-0221/11/02/C02063 (2016).
- L. Storchi within the CMS Collaboration: "Impact of low-dose electron irradiation on n(+) p silicon strip sensors", NUCLEAR INSTRUMENTS and METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT, DOI: 10.1016/j.nima.2015.08.026 (2015).
- Lorian Storchi, Roberto Paciotti, Nazzareno Re, Alessandro Marrone, "Investigation of the molecular similarity in closely related protein systems: The PrP case study" Proteins: Structure, Function, and Bioinformatics, DOI: 10.1002/prot.24836 (2015).
- Sergio Rampino, Lorian Storchi and Leonardo Belpassi, "Gold-superheavy-element interaction in diatomics and cluster adducts: A combined four-component Dirac-Kohn-Sham/charge-displacement study", Journal of Chemical Physics DOI: 10.1063/1.4926533 (2015).
- L. Storchi, F. Nunzi, F. De Angelis, "Modeling Mesoporous Nanoparticulated TiO₂ Films through Nanopolyhedra Random Packing", Journal of Physical Chemistry C, DOI: 10.1021/acs.jpcc.5b01620 (2015).
- S. Rampino, L. Belpassi, F. Tarantelli, and L. Storchi, "Full Parallel Implementation of an All-Electron Four-Component Dirac-Kohn-Sham Program", Journal of Chemical Theory and Computation, DOI: 10.1021/ct500498m (2014).

- F. Nunzi, L. Storchi, M. Manca, M. Giannuzzi, G. Gigli, F. De Angelis, "Shape and Morphology Effects on the Electronic Structure of TiO₂ Nanostructures: From Nanocrystals to Nanorods", ACS Applied Materials and Interfaces DOI: 10.1021/am404293x (2014).
- Livio Fano', Gian Mario Bilei, Lorian Storchi, Andrea Valenti, Enrico Fattibene, Matteo Manzali, Davide Salomoni, Valerio Venturi, Paolo Veronesi, Hassen Riahi, Daniele Spiga, Cinzia Amici, Serenella Carota, Francesco Cirillo, Maria Laura Maggiulli, Andrea Sergiacomi, Donatella Settimi, Claudia Diamantini, Domenico Potena, Giuseppa Ribighini, Emanuele Storti, Damiano Falcioni, Daniele FanÃ, Barbara Re, "Prototyping a Cloud Ecosystem for a Regional Public Administration", PoS(ISGC2014)009, International Symposium on Grids and Clouds (ISGC) DOI: 10.22323/1.210.0009 (2014).
- Daniele Spiga, Gian Mario Bilei, Hassen Riahi, Lorian Storchi, Enrico Fattibene, Matteo Manzali, Davide Salomoni, Valerio Venturi, Paolo Veronesi, Claudia Diamantini, Domenico Potena, Laura Raffaeli, Giuseppa Ribighini, Emanuele Storti, Livio Fano', Andrea Valentini, Damiano Falcioni, Daniele FanÃ, Barbara Re, Cinzia Amici, Serenella Carota, Francesco Cirillo, Maria Laura Maggiulli, Andrea Sergiacomi, Donatella Settimi, "A Cloud-based solution for Public Administrations. The experience of the Regione Marche", PROCEEDINGS OF THE 2014 INTERNATIONAL CONFERENCE ON COLLABORATION TECHNOLOGIES AND SYSTEMS, DOI: 10.1109/CTS.2014.6867614 (2014).
- Lorian Storchi , Sergio Rampino , Leonardo Belpassi , Francesco Tarantelli , and Harry M. Quiney, "Efficient parallel all-electron four-component Dirac-Kohn-Sham program using a distributed matrix approach.II", JCTC Journal of Chemical Theory and Computation, DOI: 10.1021/ct400752s (2013).
- Francesca Nunzi, Edoardo Mosconi, Lorian Storchi, Enrico Ronca, Annabella Selloni, M. Gra"tzel, F. De Angelis, "Inherent Electronic Trap States in TiO₂ Nanocrystals: Effect of Saturation and Sintering", Energy and Environmental Science, DOI: 10.1039/c3ee24100a (2013).
- B. Sathyaprakash, ..., L. Storchi, ... et al. "Scientific objectives of Einstein Telescope", Classical and Quantum Gravity, DOI:10.1088/0264-9381/29/12/124013 (2012).
- L. Belpassi, L. Storchi, F. Tarantelli, H. M. Quiney, "Recent advances and perspectives in 4-component Dirac-Kohn-Sham calculations", Physical Chemistry Chemical Physics, DOI: 10.1039/c1cp20569b (2011).
- P. Bolognesi, A. Kivimaki, P. O'Keeffe, V. Feyer, F. Tarantelli, L. Storchi, and L. Avaldi, "Radiationless decay in the region of the 2t_{2g} and 4e_g resonances in SF₆", Journal of Chemical Physics, DOI: 10.1063/1.3559455 (2011).
- F. Milletti, L. Storchi, L. Goracci, S. Bendels, B. Wagner, M. Kansy, G. Cruciani, "Extending pK_a prediction accuracy: high-throughput pK_a measurements to understand pK_a modulation of new chemical series", European Journal of Medicinal Chemistry, DOI: 10.1016/j.ejmech.2010.06.026 (2010).
- L. Storchi, L. Belpassi, F. Tarantelli, A. Sgamellotti, H. M. Quiney, "An efficient parallel all-electron 4-component Dirac-Kohn-Sham program using a distributed matrix approach". Journal of Chemical Theory and Computation, DOI: 10.1021/ct900539m (2010).
- F. Tarantelli, L. Belpassi, L. Storchi, "Chemical Characterization of Super-Heavy Elements by Four-Component DFT" in Parallel Computing: From Multicores and GPU's to Petascale, ed.: B. Chapman et al. p. 501-512 (IOS Press, Amsterdam) DOI: 10.3233/978-1-60750-530-3-501 (2010)
- Veronesi S., Bolognesi P., O'Keeffe P., Fainelli E., Feyer V., Prince K.C., Plekan O., Coreno M., Tarantelli F., Storchi L., Avaldi L., "Multitechnique investigation of the valence and inner shell excitation, ionization and decay of halogenated pyrimidines", Journal of Physics: Conference Series, DOI: 10.1088/1742-6596/194/2/022057 (2009)

- M. Elshakre, L. Storchi, T. Kloda, P. Linusson, F. Heijkenskjold, A. Gengelbach, L. Karlsson, T. Hansson, F. Tarantelli, R. Feifel, "A photoelectron and double photoionization study of the valence electronic structure of 1,4-bromofluorobenzene", *The Journal of Chemical Physics*, DOI: 10.1063/1.3257678 (2009).
- Cruciani G., Milletti F., Storchi L., Sforza G., Goracci L., "In silico pK(a) Prediction and ADME Profiling", *Chemistry and Biodiversity*, DOI: 10.1002/cbdv.200900153 (2009).
- F. Milletti, L. Storchi, G. Cruciani, "Predicting Protein pKa by Environment Similarity", *PROTEINS: Structure, Function, and Bioinformatics*, DOI: 10.1002/prot.22363 (2009).
- L. Storchi, G. Vitillaro, F. Tarantelli, "Implementation and use of a direct, partially integral-driven non-Dyson propagator method for molecular ionisation", *Journal of Computational Chemistry*, DOI: 10.1002/jcc.21104 (2009).
- K. Gokhberg, V. Vysotskiy, L. S. Cederbaum, L. Storchi, F. Tarantelli, V. Averbukh, "Molecular photoionization cross-sections by Stieltjes-Chebyshev moment theory applied to Lanczos pseudospectra", *The Journal of Chemical Physics*, DOI: 10.1063/1.3073821 (2009).
- F. Milletti, L. Storchi, G. Sforza, S. Cross, G. Cruciani, "Tautomer Enumeration and Stability Prediction for Virtual Screening on Large Chemical Databases", *Journal of Chemical Information and Modeling*, DOI: 10.1021/ci800340j (2009).
- P. Linusson, L. Storchi, F. Heijkenskjold, E. Andersson, M. Elshakre, B. Pfeiffer, M. Colombet, J.H.D. Eland, L. Karlsson, J.-E. Rubensson, F. Tarantelli, and R. Feifel, "Double photoionisation of thiophene and bromine substituted thiophenes", *The Journal of Chemical Physics*, DOI: 10.1063/1.3039082 (2008).
- L. Storchi and F. Tarantelli, S. Veronesi, P. Bolognesi, E. Fainelli, and L. Avaldi, "The Auger spectroscopy of pyrimidine and halogen-substituted pyrimidines", *The Journal of Chemical Physics*, DOI: 10.1063/1.2993317 (2008).
- F. Milletti, L. Storchi, G. Sforza, G. Cruciani, "New and original pka prediction method using of GRID molecular interaction fields", *Journal of Chemical Information and Modeling*, DOI: 10.1021/ci700018y (2007).
- R. Feifel, J.H.D. Eland, L. Storchi, F. Tarantelli, "An experimental and theoretical study of double photoionization of CF₄ using time-of-flight photoelectron-photoelectron (photoion-photoion) coincidence spectroscopy", *The Journal of Chemical Physics*, DOI: 10.1063/1.2386154 (2006).
- P. Bolognesi, M. Coreno, L. Avaldi, L. Storchi, F. Tarantelli, "Site-selected auger electron spectroscopy of N₂O", *The Journal of Chemical Physics*, DOI: 10.1063/1.2213254 (2006).
- L. Storchi, F. Tarantelli, A. Lagana', "Computing molecular energy surfaces on a grid", *Lecture Notes in Computer Science*, DOI: 10.1007/11751540_71 (2006).
- R. Feifel, J. H. D. Eland, L. Storchi, F. Tarantelli, "Complete valence double photoionization of SF₆", *The Journal of Chemical Physics*, DOI: 10.1063/1.2137311 (2005).
- V. Feyer, P. Bolognesi, M. Coreno, K.C. Price, L. Avaldi, L. Storchi, F. Tarantelli, "Effects of nuclear dynamics in the low kinetic energy Auger spectra of CO and CO₂", *The Journal of Chemical Physics*, DOI: 10.1063/1.1872837 (2005).
- L. Belpassi, L. Storchi, F. Tarantelli, A. Sgamellotti, H. M. Quiney, "Parallelization of a relativistic DFT code", *Future generation of computer system*, DOI: 10.1016/j.future.2003.11.016 (2004).
- L. Storchi, C. Manuali, O. Gervasi, G. Vitillaro, A. Lagana', F. Tarantelli, "Linear algebra computation benchmarks on a model grid platform", *Lecture Notes on Computer Science*, DOI: 10.1007/3-540-44862-4_32 (2003).

Design Study

- L. Storchi within the Einstein Gravitational Telescope Collaboration, "Einstein gravitational wave Telescope conceptual design study", ET-0106C-10, Issue: 4, Date: June 28, (2011). URI: <https://tds.ego-gw.it/ql/?c=7954>
- L. Storchi with the CMS collaboration, The Phase-2 Upgrade of the CMS Tracker, Technical Design Report, 2017 <https://cds.cern.ch/record/2272264?ln=en>

Technical Reports

- GEMS EXPRESSION OF INTEREST FOR THE EGI, EUDAT AND INDIGO-DATACLOUD H2020 PROJECT PROPOSAL EINFRA12 (A) Antonio Laganà, Sergio Rampino, Lorian Storchi, Ernesto Garcia, Cecilia Coletti, Edward Blurock, Carles Bo, Mirco Mariotti, Giuseppe Vitillaro
- L. Storchi, L. Belpassi, F. Tarantelli, A. Sgamellotti, H. M. Quiney, Parallelization of a relativistic DFT, Science and Supercomputing at CINECA - Report, 212 (2005).
- Laganà, F. Tarantelli, O. Gervasi, L. Pacifici, C. Villani, L. Storchi, D. Bellucci, Demonstrators and Benchmarking, ASI-PQE2000 Deliverable WP4.005-6, March 2002.
- Laganà, F. Tarantelli, O. Gervasi, L. Pacifici, C. Villani, L. Storchi, D. Bellucci, Demonstrators and Benchmarking, ASI-PQE2000 Deliverable WP4.007, July 2002.
- Laganà, F. Tarantelli, O. Gervasi, L. Pacifici, C. Villani, L. Storchi, D. Bellucci, Demonstrators and Benchmarking, ASI-PQE2000 Deliverable WP4.004, January 2002.
- Laganà, F. Tarantelli, O. Gervasi, L. Pacifici, C. Villani, L. Storchi, G. Serazzi, L. Mattoni, P. Cremonesi, P. Mori, Demonstrators and Benchmarking, ASI-PQE2000 Deliverable WP4.003, September 2001

Proceedings

- R. Di Staso, L. Aragão, E. Ronchieri, L. Storchi, D. Spiga, S. Cutini, D. Salomoni, P. Lubrano, "TIME SERIES ANALYSIS OF METEOROLOGICAL PARAMETERS AND AIR POLLUTION CONCENTRATIONS IN EMILIA-ROMAGNA, ITALY, DURING COVID-19 INFECTION", 21st International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes, HARMO 2022 , 152-156, 2022.
- Guglielmo D'Amico, Filippo Petroni, Philippe Regnault, Stefania Scocchera, Lorian Storchi, A copula based Markov Reward approach to the credit spread in European Union, 19th Applied Stochastic Models and Data Analysis International Conference (ASMDA2019)
- Mariangela Agamennone, Roberto Paciotti, Lorian Storchi, Federica Sommonte, Alessandro Marrone, "DRUGGING THE UNDRUGGABLE: THE PRION PROTEIN AS A CASE STUDY OF AGGREGATING PROTEINS", CDDD 2019
- Matteo de Santis, Lorian Storchi, Francesco Tarantelli, Leonardo Belpassi, "Charge-displacement analysis: a simple tool to reveal charge transfer effects throughout the whole periodic table (from Helium to Oganesson)", 2018
- Carla Maria Coppola, Alessandro Marrone, Cecilia Coletti, Iogann Tolbatov, Lorian Storchi, Nazzareno Re, Pietro Di Profio, Gaastra Nedea S.V., Ionut Claudiu Tranca, Silvia V. Nedea, Simone

- Arca, Emilio D'Alessandro, J. Longo, "Hydrates and Mofs as candidate Materials for Hydrogen Storage in Telecommunication Satellites", Space Propulsion 2018
- Guglielmo D'Amico, Filippo Petroni, Philippe Regnault, Stefania Scocchera and Lorian Storchi, Investigating the financial risk: information theory and break detection approach, AMASES 2018
 - Marrone A, Paciotti R, Re N, and Storchi L. A computational workflow to investigate the molecular interaction properties and aggregation propensity of prion proteins. Prion20128
 - Leonardo Belpassi, Lorian Storchi, "Bond analysis in the four-component relativistic framework: Charge-Displacement analysis via natural spinors for chemical valence", REHE2017 12th International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics
 - Guglielmo D'Amico, Stefania Scocchera, Lorian Storchi, "Financial Risk Distribution in European Union", 17th Applied Stochastic Models and Data Analysis International Conference with Demographics Workshop ASMDA2017
 - L. Storchi, F. Nunzi, S. Fantacci, F. De Angelis, "Modeling dye-sensitized TiO₂ interfaces in dye-sensitized solar cells models", SimOEAP, International Conference on Simulation of Organic Electronics and Photovoltaics, 10-14 June 2012, Spain.
 - Gabriele Cruciani, Francesca Milletti, Lorian Storchi, Gianluca Sforna, "Do pKa predictions matter anymore?", QSAR 2008, Uppsala, Sweden.
 - P. Linusson, L. Storchi, F. Heijkenkjld, E. Andersson, M. Elshakre, J.H.D. Eland, L. Karlsson, M. Larsson, J.-E. Rubensson, F. Tarantelli and R. Feifel, "Double photoionisation of thiophene and bromine substituted thiophenes", International workshop on photoionization, 2008, Uppsala, Sweden.
 - F. Milletti, L. Storchi, G. Cruciani, "New tools for pKa prediction: from small molecules to proteins", proceedings of Drug Discovery and Selection, International Conference on Medicinal Chemistry 2007, Lille, France.
 - F. Milletti, L. Storchi, G. Sforna, G. Cruciani, "A new software for pKa predictions", Proceedings of TUMA 2006, Camerino, Italy.
 - Leone B. Bosi, Lorian Storchi, "Impact of GPU Technology on gravitational wave physics and signal detection systems", E4 Workshop 2010, Bologna, Italy, 16-17 September 2010.
 - Alessandro Marrone, Lorian Storchi, Gianpiero Marconi, Emidio Albertini, The gene APOSTART: theoretical and computational study of the binding domain of phytosterols, "Chemistry Innovation and ...", University Chieti-Pescara 14 May 2013

Presentation at Conferences and Workshops

- **Invited speaker at:** Accademia dei Lincei, Rome, Quantum chemistry and cheminformatics - 26-27 September 2024, "Machine and Deep Learning techniques in chemistry: an overview from DeepGRID to a simple formula generator"
- **Invited speaker at:** University Perugia, Dpt. Chemistry, "Machine and Deep Learning techniques in chemistry: an overview from DeepGRID to a simple formula generator", May, 2024
- **Invited speaker at:** VISTEC Vidyasirimedhi Institute of Science and Technology, School of Molecular Science and Engineer 31/05/2022 (Thailand)
- **Invited speaker at:** Shoolini Science Web Series Lecture IX - "Four-component Dirac-Kohn-Sham Calculations" 30/06/2021
- "Machine and Deep Learning techniques in chemistry: from DeepGRID to a simple formula generator", Southern European Conference on the Science of Molecules Perugia, 27-29 September 2023

- “Applications of Machine and Deep Learning techniques: from DeepGRID to a simple formula generator”, Center for Advanced Studies and Technology University «G. d’Annunzio», Chieti-Pescara, December 19, 2023
- *BERTHA and PyBERTHA: State of the Art for Full Four-Component Dirac-Kohn-Sham Calculations. PARCO 2019: 354-363.*
- “Machine and Deep Learning techniques in chemistry: from DeepGRID to a simple formula generator”, Experiment-Theory: a round trip, Chieti, Sept 14th 2023
- “The Track Fitter for L1 Tracking”, First H-Team Workshop - Higgs precision physics at LHC with Trigger, Electronics and Advanced Methods Thursday 07 April 2016 – Friday 08 April 2016 Cortona – Italy
- “Computing molecular energy surfaces on a grid”, (ICCSA06), Glasgow, 8-11 May 2006.
- “SUPSIM: Computing electronic potential energy surfaces on a GRID”, Tutorial on grid technologies, (ICCSA04), Assisi, 13-14 May 2004
- “Computing electronic PES on a GRID”, V Edizione del Congresso del Gruppo Italiano di Chimica Computazionale, Siena, 6-18 December 2003

Congress organization

- **Co-Chair** of the REHE – 2020/2022 - 13th International Conference on Relativistic Effects in Heavy-Element Chemistry and Physics, Assisi - Italy (2022) <https://www.rehe2020.it/>
- Part of the organizing committee of the MES 2024 - Molecular Electronic Structure 2024, Pescara - Italy, 2024 <https://www.mes2024.it/>
- Part of the organizing committee of the HOPV 2010 - International Conference on Hybrid and Organic Photovoltaics, Assisi - Italy, 2010

Schools

- “Summer School of Advanced Calculus - Second Edition”, Castel Gandolfo (Roma), 28 agosto – 8 September 2006.
- “First Specialization School on Parallel Computing”, CINECA Casalecchio di Reno (Bologna), 24-28 October 2005.
- “The 2nd International Summer School on grid computing 2004”, Vico Equense (Napoli), 18-30 July 2004

Workshops and Tutorials

- “ICT security Day 2012”, University of G. D’Annunzio Chieti-Pescara.
- “NVIDIA Cuda Workshop”, Roma, Institute of Applied Mathematics (CNR), 19-20 July 2010.
- “Modeling Winter 2010”, Pisa, Scuola Normale Superiore, February 26, 2010
- “HPC with CUDA”, Department of Electrical Systems and Automation of the University of Pisa, September 7, 2009.

- "Developing for Multi-core Intel seminar", Roma, Italy, November 20, 2008
- "Joint ICTP-KFAS Workshop on Nanoscience for Solar Energy Conversion", ICPT, Trieste, Italy, 27-29 October 2008.
- "Cluster OpenMP Workshop", CASPUR, Roma, December 7, 2006.
- "QCDOC and BlueGene Workshop Next generation of HPC architectures", EPCC, Edinburgh, 4-6 October 2005.
- "ASSIST Tutorial", Department of Computer Science University of Pisa, 5-7 May 2004.
- "ENACTS (European Network for Advanced Computing Technology for Science) 4rd Annual Meeting", Prague, 11-13 March 2004.
- "Tutorial on Grid Computing", Swiss National Supercomputing Center, 25-26 October 2003.
- "ENACTS (European Network for Advanced Computing Technology for Science) 3rd Annual Meeting", Dublin, 14-15 March 2003.
- "Performance Tuning for Microprocessor-Based Systems Workshop", CINECA Casalecchio di Reno (Bologna), January 17, 2002
- "INFN-GRID/EDG User Tutorial", Turin, 5-6 December 2002.
- I also participated with numerous contributions to workshops conducted within the projects: "ASIPQE2000", "GRID.IT".
- "High Performance Computing in Chemistry", NNL, Lecce, 2009.

Periods of study abroad and Invited Professor

- **Invited Professor:** "Université de Lorraine, 54000 Nancy" at the "Laboratoire de Physique et Chimie Théoriques (UMR) CNRS", Academic Year 2021/22
- Heidelberg (Germania) at: "Physikalisch-Chemisches Institut (Theoretische Chemie)". February-March 2005 and April - May 2006
- Budapest (Ungheria) at: "MTA SZTAKI - Computer and Automation Research Institute of the Hungarian Academy of Sciences", "The Chemical Research Center of the Hungarian Academy of Sciences (CRC HAS)". November - December 2004

Awards

- Member of the BondMachine project that has been granted an Iron Medal at the Innovate FPGA 2018 grand final (<http://www.innovatefpga.com>, under the name Reconfigurable Computing). Part of the presenter team at Intel San Jose, CA, USA (2018)
- Awarded with a consultancy contract (consultancy topic: Machine and Deep Learning techniques) within the project VITALITY at the University of Perugia (2024/2025).

Teaching

- Teacher at the Multiscale, Machine Learning and QSAR methods applied to biomolecules: “Introduction to Machine and Deep Learning using python”, Aspet, France, 25-29, November, 2024
- Material Chemistry, Corse Degree in Biomedical Engineering, (University of Chieti-Pescara) - starting from Academic Year 2021/22 up to now
- Basics of computer science - Corse Degree in TESTA (University of Chieti-Pescara) - starting from Academic Year 2021/22 up to now
- General Chemistry - Corse Degree in TESTA (University of Chieti-Pescara) - starting from Academic Year 2021/22 - 2022/23 up to now
- Statistics and computer science - Course Degree in TPALL (University of Chieti-Pescara) - starting from Academic Year 2014/2015 up to now
- Computational Chemistry, Course Degree in C.T.F (University of Chieti-Pescara) - starting Academic Year 2018/19 up to Academic Year 2021/22
- Computer programming & Data Analysis using Python - PhD Course Degree Business and Behavioural Sciences (University of Chieti-Pescara) - starting from Academic Year 2016/2017 up to now
- Introduction to Chemo and Bioinformatics - Course Degree in C.T.F (University of Chieti-Pescara) - starting from Academic Year 2015/2016 up to 2016/17
- General Chemistry - Course Degree in TPALL (University of Chieti-Pescara) - starting from Academic Year 2014/2015 up to 2019/20
- General Chemistry - Course Degree in Assistenza Sanitaria - (University of Chieti-Pescara) - starting from Academic Year 2015/2016 up to 2016/2017
- General and Inorganic Chemistry - Course Degree in Pharmacy (University of Chieti-Pescara) - starting from Academic Year 2012/2013 up to 2019/20
- General and Inorganic Chemistry - Course Degree in C.T.F. (University of Chieti-Pescara) - Academic Year 2011/2012 (20 hours)
- Computational Chemistry - Course Degree in C.T.F. (University of Chieti-Pescara) – Academic Year 2014/2015 (few hours) - Academic Year 2015/2016 - 2016/2017
- Advanced Computational Methods - Course Degree in Computer Science (University of Perugia) - starting from Academic Year 2010/2011 up to 2011/2012
- Applications and Computing with Network - Course Degree in Computer Science (University of Perugia) - starting from Academic Year 2007/2008 up to 2010/2011
- Applications and Computing with Network II - Course Degree in Computer Science (University of Perugia) - Academic Year 2005/2006
- Computer Science - Degree in Technology for Conservation and Restoration of Cultural Heritage (University of Perugia) starting from Academic Year 2004/2005 up to 2007/2008
- Operating Systems Laboratory 3 - Course Degree in Computer Science (University of Perugia) - Academic Year 2005/2006
- General Laboratory of Computer Science - Course Degree in Computer Science (University of Perugia) - starting from Academic Year 2005/2006 up to 2008/2009
- Lecturer at the TCCM 06 - European Master in Theoretical Chemistry and Computational Modeling -Year 2006
- Atomic and Molecular structures - Course Degree in Computer Science (University of Perugia) -Support to teaching - Academic Year 2003/2004
- One year contract professor for the course” Applications and Computing with Networks” Degree in Computer Science University of Perugia academic year 2010/2011

Projects

- **Principal Investigator** of the “PaGUSci” project (Parallelization and GPU Porting of Scientific Codes) within the Cascading Call issued by Spoke 3 and relating to the implementation of the Research “National Centre for HPC, Big Data and Quantum Computing”
- Open City Platform (OCP) intends to research, develop and test new technology solutions that are open, interoperable and usable on-demand on the Cloud, as well as innovative organizational models that will be sustainable over time. The aim of the project is to innovate, with scientific results and new standards the delivery of services by Local Government Administrations (LGA).
- ASI-PQE2000 within that project I developed and integrated methods for the dynamic allocation of memory in the framework of ASSIST.
- GRID.IT (technical board member) within the project I worked mainly of the activity about ChemGrid.
- ChemGrid I worked as a project coordinator, giving the basis and guidelines for its realization.
- LIGTHS (LIgand to interfere with Human TS).
- DEISA Project” Chemical Characterization of Super Heavy Elements (E112 and E114) by 4-component relativistic DFT.”
- Many-cores Computing for future Gravitational Observatories (MaCGO). Within this project I worked mainly in developing the basic structure of a general purpose library for computation using many cores environment.
- H-team The discovery of the Higgs boson opens de-facto’ the phase of the precision measurement of its couplings. The aim of this research project is to develop the most advanced trigger, selection and analysis techniques to allow the LHC experiments to gain an order of magnitude with respect to the current levels of accuracy. In such a way it would become possible to explore the existence of new physics over a wide energy regime.

Posters

- ”Chemical Characterization of Super Heavy Elements by four-component relativistic DFT. (CC-SHE)”, Leonardo Belpassi, Lorian Storchi, Francesco Tarantelli, Molecular Properties 2009, Oslo.
- ”Chemical Characterization of Super Heavy Elements by four-component relativistic DFT. (CC-SHE)”, Leonardo Belpassi, Lorian Storchi, Francesco Tarantelli, DEISA Meeting 2009.
- ”An all-electron 4-component Dirac-Kohn-Sham procedure for large molecules and clusters containing heavy elements.” Leonardo Belpassi, Francesco Tarantelli, Antonio Sgamellotti, Lorian Storchi, Harry M. Quiney, ”Joint ICTP-KFAS Workshop on Nanoscience for Solar Energy Conversion”, ICPT, Trieste Italy, 27-29 Ottobre 2008.
- ”Characterization of inner shell excitation, ionization and decay of pyrimidine”, S. Veronesi, P. Bolognesi, E. Fainelli, V.Feyer, K.C.Prince, P.O.Kudelic, M.Coreno, F. Tarantelli, L. Storchi and L. Avaldi., IX School on Synchrotron Radiation: Fundamentals, Methods and Applications, 2007
- ”New tools for pKa prediction - from small molecules to proteins” F. Milletti, L. Storchi, G. Sforza, G. Cruciani. Drug Discovery and Selection, International Conference on Medicinal Chemistry 2007, Lille, France.

- "MoKa - pKa prediction software", M. Shalaeva, Z. Zhu, R. Stanton, D. Li, F. Milletti, L. Storchi, G. Sforza, G. Cruciani. Euro QSAR 2006, Italy, 10-16 September 2006.
- "Parallelization of a relativistic DFT code", L. Belpassi, L. Storchi, F. Tarantelli, A. Sgamellotti, H. M. Quiney. V Edition of the Congress of the Italian Group of Computational Chemistry, Siena, 6-18 December 2003

Thesis Supervisor

- Matteo Picciolini, "Postprocessing and Display in theoretical simulations of Molecular Spectroscopy", University of Perugia, Course Degree in Computer Science, Supervisors: Francesco Tarantelli, Lorian Storchi
- Francesco Muscarà, "DHCP: virtualization and management", University of Perugia, Course Degree in Computer Science, Supervisors: Francesco Tarantelli, Lorian Storchi
- Andrea Lauri, "Using ScaLAPACK and Adaptive MPI in a Relativistic DFT code", University of Perugia, Course Degree in Computer Science, Supervisors: Francesco Tarantelli, Lorian Storchi
- Daniele Bocciolini, "Use and management of SMARTCARD for authentication procedures", University of Perugia, Course Degree in Computer Science, Supervisors: Francesco Tarantelli, Lorian Storchi
- Matteo De Bonis, "Pseudo-Random number generators on GPU", University of Perugia, Course Degree in Computer Science, Supervisors: Leonello Servoli, Lorian Storchi, Leone Bosi
- Fabio Andrea Petrini, "Authentication, Authorization, Accounting for a secure wireless network" University of Perugia, Course Degree in Computer Science, Supervisors: Francesco Tarantelli, Lorian Storchi
- Lanfranco Fontana, "Using MPI and Pthreads for parallelization on multi-GPU platform of gravitational signals identification algorithms" University of Perugia, Course Degree in Computer Science, Supervisors: Leonello Servoli, Lorian Storchi, Leone Bosi
- Matteo Picciolini, "GPGPU and multithreading in molecular ionization spectra computation" University of Perugia, Course Degree in Computer Science, Supervisors: Francesco Tarantelli, Lorian Storchi
- Antonio Nigro, "Study and implementation of algorithms for spheres packing in Simulation of nanoporous materials" University of Perugia, Course Degree in Computer Science, Supervisors: Francesco Tarantelli, Lorian Storchi
- Andrea Lauri, "Development of a gesture controller for a Python molecular visualization system", University of Perugia, Course Degree in Computer Science, Supervisors: Francesco Tarantelli, Lorian Storchi, Massimiliano Pippi
- Ermanna Fabbri, "Algorithms for the packing of spheres and polyhedra in the simulation of nanoporous materials of potential pharmaceutical interest", University of Chieti-Pescara, Course degree in Pharmacy, Supervisors: Lorian Storchi
- Matteo Pergolesi, "Design and implementation of a monitoring system for federated cloud infrastructure", University of Perugia, Course degree in Computer Engineering, Supervisors: Prof. Gianluca Reali, Dr. Lorian Storchi
- Gabriele Galli, "AI-based intelligent caching system for the CMS experiment", University of Perugia, Course degree in Physics, Supervisors: Prof. Lorian Storchi, Prof. Livio Fanò, Dr. Daniele Spiga
- Giandomenico Terrenzio, "Study, use and implementation of numerical procedures (Machine Learning algorithms) for the prediction of the logD of molecular structures of potential chemical-pharmaceutical interest", University of Chieti-Pescara, Course degree in CTF, Supervisors: Prof. Lorian Storchi

- Giacomo Surace, "FPGA accelerators userspace library development", University of Perugia, Course Degree in Computer Science, Supervisors: Giovanni Ambros, Mirko Mariotti, Lorian Storchi
- Luna Di Marco, "PROCESSES AND CHEMICAL COMPOSITIONS FOR STORAGE IMPROVED MOLECULAR HYDROGEN IN HYDRATE CLATHRATES", Pietro Di Profio, Lorian Storchi
- Giuseppe Prudente, "Use of Machine Learning techniques to study the possible role of air pollutants in the spread of COVID-19", University of Perugia, Corse degree in Physics, Supervisors: Prof. Lorian Storchi, Prof. Livio Fanò, Dr. Daniele Spiga

Tutor (Stages)

- Matteo De Bonis, "Test and porting of code on GPU", at INFN Perugia.
- Metteo Picciolini, "Implementation of a url shortening service by the development environment provided by google apps using python language", at Evonove s.r.l.
- Antonio Nigro, "Implementation using Python language of an online system storing on Google Blobstore backend including client desktop in a transparent manner that supports the symmetric key encryption methodology", st Evonove s.r.l.
- Andrea Lauri, "Construction of a gesture-based controller using Microsoft Kinect device", at Evonove s.r.l.



Firmato digitalmente da Lorian Storchi
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