

Prof. Ester Chiessi. Update March 2022

Education and Research Appointments:

1978: Secondary School (Humanities) Graduation (60/60)

1984: Graduation in Chemistry at the University of Rome "La Sapienza" (110/110 cum laude)

1984 - 1986: Researcher at CSM (Centro Sviluppo Materiali, Material Development Centre, Pomezia, Rome)

1987: Chemistry Teaching Qualification in Secondary Schools (classes A013, A060)

1989: Ph.D. Graduation in Chemistry at the University of Rome "La Sapienza"

1989-2020: Researcher in Physical Chemistry, Department of Chemical Sciences and Technologies, University of Rome Tor Vergata

2018: National Scientific Qualification of Associate Professor (03/A2).

2021-: Associate Professor in Physical Chemistry, Department of Chemical Sciences and Technologies, University of Rome Tor Vergata

Memberships:

Società Chimica Italiana; Consorzio Nazionale Interuniversitario per le Scienze Fisiche della Materia, CNISM; National Interuniversity Consortium of Materials Science and Technology, INSTM; National Interuniversity Consortium of Biostructures and Biosystems, INBB.

Associate researcher of the Institute of Complex Systems of CNR, Rome, since 2018.

Editor of *Journal of Chemistry* and *Journal of Soft Matter* (Hindawi Publishing Corporation) 2013-2021.

Peer Reviewer for *Physical and Macromolecular Chemistry Journals* of American Chemical Society, Elsevier, Wiley, MDPI, Royal Society of Chemistry since 2007.

Recognised by the editors as an Outstanding Reviewer for *RSC Advances* in 2020.

Reviewer for MIUR since 2012.

Invited reviewer for the CINECA ISCRA initiative.

Invited external reviewer/rapporteur for the Romanian National Research Council (Calls: PCE-2012, PCE-2016, Postdoctoral research and Young research teams Projects 2019, PCE 2021, TE 2021, PD 2021).

Invited speaker at the online conference on "Osmolyte and cosolvent effects in stimuli-responsive soft matter systems" February 25-26, 2021.

Award

2018: Selection of the paper 'On the molecular origin of the cooperative coil-to-globule transition of poly(N-isopropylacrylamide) in water' by L. Tavagnacco, E. Zaccarelli and E. Chiessi, *Phys. Chem. Chem. Phys.*, 2018, 20, 9997-10010, as a "key scientific article contributing to excellence in science and engineering research" by the Advances in Engineering selection committee <https://advanceseng.com/pnipam-molecular-thermosensitive-synthetic-macromolecule-water/>

Current Research Activity

The research interests are focussed on the study of structural and functional properties of biopolymers and of biocompatible synthetic polymer systems in solution and in gel phase. Molecular modeling methods are applied to elucidate structural and dynamical properties, such as the conformational preferences of the glycosidic linkages and the role of the molecular flexibility in conformational transitions of polysaccharides.

The dynamics of non reactive processes in polymer hydrogels, such as chains fluctuations, network responsivity to environmental stimuli and water diffusion, and influence of cross-links density and macromolecular scaffold hydrophobicity on the hydrogel nanostructure are investigated by

molecular dynamics and metadynamics simulations, with the support of spectroscopy, rheology, dynamic light scattering and confocal fluorescence microscopy techniques.

Incoherent quasi-elastic and elastic neutron scattering experiments, performed at European scattering facilities, are carried out to study water and polymer features in microgels.

Principal investigator of 21 projects funded by National Supercomputing Facilities CASPUR or CINECA.

Participant of 5 European Projects (within the 6th and 7th Framework Program and Horizon 2020, including “AMPHORA, Acoustic Markers for Enhanced Remote Sensing of Radiation Doses” European Union Project, Programme Funding: Horizon 2020, Sub Programme Area: FETOPEN-1-2016-2017; “Modeling Microgels: MIMIC” ERC Consolidator Project 2016-2020; “Theraglio: developing theranostics for gliomas” European Union Project, Seventh Framework Programme FP7/2007-2013) and of several National Projects.

Authoring Activity

72 Scientific Contributions on International Journals and Books of Physical and Macromolecular Chemistry (Scopus & Web of Science). H index = 26 (Scopus). Number of citations: 2119. 2010-2020 decade Journal Impact Factor (per Product): 4.04

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Teaching Activity

Chemical Thermodynamics and Kinetics, Laboratory of Physical Chemistry: 1995-2016; Chemistry of Macromolecules since 2017; Biophysical Chemistry since 2022.

Thesis supervision (co-supervision) of 10 (6) undergraduate students (2004-2021).

Books:

CHIESSI E, PARADOSSI G (2009). Problemi di Chimica Fisica.

ROMA: Universitalia, ISBN: 978-88-95244-49-5.

CHIESSI E, PARADOSSI G (2011). Problemi di Chimica Fisica. Seconda Edizione. p. 1-412,

ROMA: Universitalia, ISBN: 978-88-65071-13-7.

Member of 2 PhD Thesis Committees (2010, 2011).

Member of the Committee of PhD School in Chemical Science of the University of Rome Tor Vergata: 2013-2018. Lecturer for the PhD School in Chemical Science of the University of Rome Tor Vergata: 2019-2020.

Member of the Lecturer-Student Committee (Commissione Paritetica Docenti-Studenti) of the Department of Chemical Science and Technologies: 2013-2020.

Scientific dissemination.

Webmaster of:

<http://www.stc.uniroma2.it/cfmacro/cfmacroindex.htm>

Current and Recent Projects

Principal Investigator

“Insulin In-silico Lyophilisation: InsInsLy”

CINECA ISCRA C 2022

“Tuning thermoresponsIvity of aMphihilic polymErs: TIME”
CINECA ISCRA C 2021

“Mechanical properties simUlationS of polymer architectures: MUSIC”
CINECA ISCRA C 2020

“In-Silico DEformation of polymer networks: ISIDE”
CINECA ISCRA C 2019

“APOferritin, LYSozyme and INsulin in the amorphous state at low hydration: APOLYSIN”
CINECA ISCRA C 2019

“ETHanol Influence on lower Critical Solution temperature behaviour of poly(n-isopropylacrylamide): ETHICS”
CINECA ISCRA C 2018

“Simulations of Proteins in lYophilised state: SPY”
CINECA ISCRA C 2017

“SImulations of polymer MIcrogels at Low wAtEr content: SIMILAR”
CINECA ISCRA C 2016

“Surface Interactions Between poly-N-isopropylacrYLamide microgels: SIBYL”
CINECA ISCRA C 2016

“Interchain Interactions in Poly(N-isopropylacrylamide) Aqueous SolutionS: II-PASS”
CINECA ISCRA C 2015

“Tacticity Influence on Thermo-responsivity of poly(N-IsopropylACrylamide): TITANIC”
CINECA ISCRA C 2014

“Simulation Tests of Rheological Experiments in Soft Systems: STRESS”
CINECA ISCRA C 2013

“Solution behaviour of poly(vinyl alcohol): a molecular dynamics simulation study”
CASPUR Standard HPC Grant 2012

“Focussing on poly(vinyl ALcohol) Simulations to Test Accurate Force Fields: FALSTAFF”
CINECA ISCRA C 2011

“Simulations of Interfaces in polymer MicroBalloons with Atomic Detail: SIMBAD”
CINECA ISCRA C 2010

“Molecular Dynamics Simulation Study of Thermosensitive Polymer Hydrogels”
CASPUR Standard HPC Grant 2009

“Structure and Dynamics of Amphiphilic Polymer Networks with a High Hydration Degree”
Supercomputing Project 2008 - CNISM-CINECA. Physics of Matter

"Molecular Dynamics Simulation Study of the Hydrogels of HYADD4, a Hyaluronic Acid Derivative" Computing Project funded by CASPUR (2007-08)

"Molecular Dynamics Simulations of Amphiphilic Polymeric Aggregates in Aqueous Solution" Supercomputing Project 2007 - CNISM-CINECA. Physics of Matter

"Dynamics Simulations of Amphiphilic Chemical Hydrogels Based on Poly-(vinyl alcohol)" CINECA Supercomputing Project 2006 - Physics of Matter

"Dynamics of confined water in poly-(vinyl alcohol) hydrogels: simulation and experiment" CINECA-INSTM co-funded Computing Project (2004-2005)

Partecipant

“MICROARTE”

Funded by Regione Lazio – Bando Gruppi di Ricerca 2020

“GlioBubbles – Glioma Targeting by Drug Loaded Engineered Microbubbles”

Funded by Ministero degli affari esteri e della cooperazione internazionale 2021-2022

“GELARTE: Microgel e arte: una nuova tecnologia per la conservazione dei beni cartacei”

Funded by LAZIO INNOVA – Regione Lazio 2018/2020

“AMPHORA, Acoustic Markers for Enhanced Remote Sensing of Radiation Doses”

European Union Project, Programme Funding: Horizon 2020, Sub Programme Area: FETOPEN-1-2016-2017

“Modeling Microgels: MIMIC”

ERC Project 2016-2020

“AcouGraph”

Funded by the University of Rome Tor Vergata within the Programme Consolidate the Foundations 2015

“Theraglio: developing theranostics for gliomas”

European Union Project, Seventh Framework Programme FP7/2007-2013

“3MiCRON: MultiModality MicroBalloons”

European Project within the NMP theme of the 7th Framework Program of the European Commission

“S.I.G.H.T.: Systems for in-situ theranostics using micro-particles triggered by ultra-sound”

European Project within the IST priority 2.5.2. of the 6th Framework Program of the European Commission

“Physical and chemical characterization of viscosupplements based on Hyaluronic acid”

Project Funded by FIDIA Farmaceutici S. p. A. 2009-2010; 2011-2012; 2013-2014