

– ANDREA TAGLIABUE, PhD –

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– EDUCATION AND RESEARCH EXPERIENCE –

- 2012–2014 Università degli Studi dell'Insubria, **Bsc.: Chemistry and Industrial Chemistry**
Thesis: *Coarse-grained Numerical Simulations of Out-of-Equilibrium Phenomena: Self-Assembly of Anisotropic Nanoparticles.*
Advisor: Massimo Mella, Prof.
- 2015–2017 Università degli Studi dell'Insubria, **Msc.: Chemistry**
Thesis: *Statistical Thermodynamics of Confined Weak Polyelectrolytes: Impact of Charged Hydrogen Bonds, Ramifications and Solution Ionic Strength on Conformations and Titration curves.*
Advisors: Massimo Mella, Prof., Dario Bressanini, PhD
- 2018–2020 Università degli Studi dell'Insubria, **PhD: Chemical and Environmental Sciences**
Thesis: *Stochastic Coarse-grained Simulations of Polyelectrolytes in Aqueous Solutions.*
Advisor: Massimo Mella, Prof.
- 2021–Present Southern Methodist University, **post-doctoral fellow**
Project: *Mesocale Simulations of Light Harvesting in Plant Photosynthetic Membranes.*
PI: Doran I. G. Bennett, Prof.

– PUBLICATIONS –

1. Mella, M., [Tagliabue, A.](#), Mollica, L., Vaghi, S., Izzo, L. **Inducing pH Control over the Critical Micelle Concentration of Zwitterionic Surfactants via Polyacids Adsorption: Effect of Chain Length and Structure (2021)**, *Journal of Colloid and Interface Science*, article in press.
2. Mella, M., [Tagliabue, A.](#), Vaghi, S., Izzo, L. **Evidences for Charged Hydrogen Bonds on Surfaces Bearing Weakly Basic Pendants: The Case of PMMA-*ran*-PDMAEMA polymeric films (2021)**, *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, 620, 126525.
3. Staño, R., Košován, P., [Tagliabue, A.](#), Holm, C. **Electrostatically Cross-Linked Reversible Gels—Effects of pH and Ionic Strength (2021)**, *Soft Matter*, 17 (5), 1574-1588.
4. [Tagliabue, A.](#), Landsgesell, J., Mella, M., Holm, C. **Can Oppositely Charged Polyelectrolyte Stars Form a Gel? A Simulational Study (2021)**, *Soft Matter*, 17 (5), 1574-1588.

- Mella, M., [Tagliabue, A.](#), Izzo, L. **On the Distributions of Hydrophilic Polyelectrolytes and Their Counterions Around Zwitterionic Micelles: The Possible Impact on the Charge Density in Solution** (2021) *Soft Matter*, 17 (5), 1267-1283
- Mella, M., [Tagliabue, A.](#), Mollica, L., Izzo, L. **Monte Carlo Study of The Effects of Macroion Charge Distribution on the Ionization and Adsorption of Weak Polyelectrolytes and Concurrent Counterion Release** (2020) *Journal of Colloid and Interface Science*, 560, 667-680.
- [Tagliabue, A.](#), Izzo, L., Mella, M. **Interface Counterion Localization Induces a Switch between Tight and Loose Configurations of Knotted Weak Polyacid Rings despite Intermonomer Coulomb Repulsions** (2020) *The Journal of Physical Chemistry B*, 124 (14), 2930-2937.
- Izzo, L., Gorrasi, G., Sorrentino, A., [Tagliabue, A.](#), Mella, M. **Controlling Drug Release of Anti-inflammatory Molecules Through a pH-Sensitive, Bactericidal Polymer Matrix: Towards a Synergic and Combined Therapy** (2020) *Lecture Notes in Bioengineering*, 151-163.
- [Tagliabue, A.](#), Izzo, L., Mella, M. **Impact of Charge Correlation, Chain Rigidity, and Chemical Specific Interactions on the Behavior of Weak Polyelectrolytes in Solution** (2019) *The Journal of Physical Chemistry B*, 123 (42), 8872-8888.
- [Tagliabue, A.](#), Izzo, L., Mella, M. **Absorbed Weak Polyelectrolytes: Impact of Confinement, Topology, and Chemically Specific Interactions on Ionization, Conformation Free Energy, Counterion Condensation, and Absorption Equilibrium** (2019) *Journal of Polymer Science, Part B: Polymer Physics*, 57 (9), 491-510.
- Cesari, C., Mazzoni, R., Matteucci, E., Baschieri, A., Sambri, L., Mella, M., [Tagliabue, A.](#), Basile, F.L., Lucarelli, C. **Hydrogen Transfer Activation via Stabilization of Coordinatively Vacant Sites: Tuning Long-Range π -System Electronic Interaction between Ru(0) and NHC Pendants** (2019) *Organometallics*, 38 (5), 1041-1051.
- [Tagliabue, A.](#), Izzo, L., Mella, M. **Out of Equilibrium Self-Assembly of Janus Nanoparticles: Steering It from Disordered Amorphous to 2D Patterned Aggregates** (2016) *Langmuir*, 32 (48), 12934-12946.

– PRESENTATIONS –

Posters:

- [Tagliabue, A.](#), Mella, M. **Out-of-equilibrium Self-Assembly of Janus Nanoparticles: Steering it from Nanostructures to 2D Patterns**, MolsSimEng 2015, Polytechnic of Milan, 18 September 2015.
- [Tagliabue, A.](#), Mella, M., Izzo, L., Mollica, M. **Weak Polyelectrolytes with Strong H-bond Interactions: Titration and Pore Adsorption Equilibria**, MIPOL2017, Milan, 15-16 February 2017.
- [Tagliabue, A.](#), Izzo, L., Mella, M. **Modulating Knots Localization in Weak Ring-Shaped Polyelectrolytes**, MIPOL2020, Milan, 15-17 July 2020.

Oral communications (the first author is the speaker):

- Mazzoni, R., Cesari, C., Cingolani, A., Zanotti, V., Cavani, F., Puzzo, F., Lucarelli, C., Mella, M., [Tagliabue, A.](#), Baker, T. **The Power of Ligand Combination in Redox Active Ruthenium and Iron Complexes**, XXVI Congresso Nazionale della Società Chimica Italiana, Paestum (Sa), 10-14 September 2017.
- [Tagliabue, A.](#), Cesari, C., Mazzoni, R., Lucarelli, C., Mella, M. **Understanding Homogeneous Hydrogenation of Polar Double Bonds Mediated by Ru(0) Complexes via DFT Calculations**, Congresso Nazionale della SCI – Divisione di Chimica Fisica, Bologna, 25-28 June 2018.

3. Mella, M., [Tagliabue, A.](#), Izzo, L. **Weak Polyelectrolytes in Brine: Effects of Chemical Specific Interactions, Topology, Salt Valency and Concentration on Conformations and $pK_a^{(eff)}$** , Congresso Nazionale della SCI – Divisione di Chimica Fisica, Bologna, 25-28 June **2018**.
4. Izzo, L., Gorrasi, G., Sorrentino, A., [Tagliabue, A.](#), **Controlling Drug Release from a pH-sensitive Polymer Matrix**, BIONAM2019, MSC Orchestra Mediterranean Sea, September 29 – October 03 **2019**.
5. Mella, M., Vaghi, S., Izzo, L., [Tagliabue, A.](#), Vigliotta, G. **Weakly Polyelectrolytic Surfaces: Are There Important Interactions Between Ionized and Neutral Tethered Monomers?**, MIPOL2020, Milan, 15-17 July **2020**.

– CERTIFICATIONS –

- “Introduction to Parallel Computing with MPI and OpenMP”, CINECA, Segrate (MI), Italy, 22-24 November 2017.
- “Introduction to Python programming”, CINECA, Segrate (MI), Italy, 04-05 April 2018.
- “Active, Charged, and Magnetic Soft Matter Simulations with ESPResSo”, CECAM summer school, ICP Stuttgart, Germany, 7-11 October 2019.

– TEACHING EXPERIENCE –

2019–2021 Lectures in "*Physical Chemistry II*" (basic principles of quantum chemistry and spectroscopy), Università degli Studi dell'Insubria.

– TECHNICAL EXPERTISE –

Fortran 77/90 | Python | ESPResSo | Gaussian 09 (post-HF, DFT, PCM) | VMD | LaTeX | Biopython
Molecular Dynamics | Monte Carlo | Advanced Sampling Methods | Photosynthesis | Light harvesting
Generalized Forster Energy Transfer

– REFERENCE CONTACTS –

Massimo Mella, Prof.
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