BIOGRAPHICAL SKETCH

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NAME: Poma, Adolfo

POSITION TITLE: Assistant Professor of Computational Modelling of Complex Systems

EDUCATION/TRAINING (*Begin with baccalaureate or other initial professional education, such as nursing, include postdoctoral training and residency training if applicable. Add/delete rows as necessary.*)

INSTITUTION AND LOCATION	DEGREE (*if applicable*)	Completion Date MM/YYYY	FIELD OF STUDY
National University of San Marcos, Lima (Peru)	B.S	04/2004	Physics
State University of Campinas, Sao Paulo (Brazil)	M.Sc.	08/2007	Statistical Physics
Johannes Gutenberg University, Mainz (Germany)	Ph.D.	05/2011	Soft Matter Physics

A. Personal Statement

I have the expertise, leadership, training and motivation necessary to successfully carry out the proposed research project. I have a broad background in computational physics, physical-chemistry and biophysics with specific focus on conformational changes of large biomolecules and particular interest in the molecular basis of COVID-19 disease. My current research includes nanomechanics studies of protein complexes with interest in biomedical applications. As PI or co-Investigator on several research institutions and national polish grants as well as Horizon 2020-funded grants, I have gathered sufficient knowledge for conducting the proposed research by developing novel computational approaches for the study of protein-protein and protein-sugar interactions by molecular dynamics simulations, energetic characterization of protein binding, and in-house methods such as Gō-Martini approach (main developer) for the sampling of large conformations in proteins, and by establishing strong ties with Martini force field community as a member of the TaskForce for proteins. In addition, I successfully managed the projects (e.g. staffing, research and budget planning), collaborated with other researchers in Europe and overseas (USA and Japan), and produced several peer-reviewed publications from each project. As a result of these previous experiences, I am fully aware of the role of frequent communication among project members and the design of a research plan, timeline, and correct budget planning. All mentioned achievements are documented in the following publications.

1. Thu, T. T. M., Moreira, R. A., Weber, S. A., & Poma, A. B. (2022). Molecular Insight into the Self-Assembly Process of Cellulose Iβ Microfibril. International Journal of Molecular Sciences, 23(15), 8505.

2. Liu, Z., Moreira, R. A., Dujmović, A., Liu, H., Yang, B., Poma, A. B., Nash, M. A. (2021). Mapping mechanostable pulling geometries of a therapeutic anticalin/CTLA-4 protein complex. *Nano letters*, **22**(1), 179–187.

3. Mahmood, M. I., Poma, A. B., Okazaki, K. I. (2021). Optimizing Gō-MARTINI coarse-grained model for F-BAR protein on lipid membrane. *Frontiers in molecular biosciences*, 8, 619381.

4. Senapati, S., Poma, A. B., Cieplak, M., Filipek, S., & Park, P. S. H. (2019). Differentiating between inactive and active states of rhodopsin by atomic force microscopy in native membranes. *Analytical chemistry*, 91(11), 7226-7235.

B. Positions, Scientific Appointments and Honors

Positions and Employment

2011–2013	Postdoc, Computational Physics, Institute of Physics, University of Rome ”La Sapienza”, Rome, Italy
2013–2018	Postdoc, Division of Biophysics, Institute of Physics, Polish Academy of Sciences, Warsaw, Poland
2018–till now	Assistant Professor, Department of Soft Matter and Biosystems, Polish Academy of Sciences, Warsaw, Poland
2021–2022	Junior Group Leader of Computational Chemistry, ICRI-BioM at Lodz University of Technology, Lodz, Poland

Other Experience and Professional Memberships

2019–	Member, Polish Physical Society
2017–	Member, Biophysical Society
2022–	Editorial Board of the Journal of Structural Biology (JSB/JSBX)
2022–2025	NCN/FNP Peer Reviewer

Honors

2022	First Quarter – Outstanding Research Award, Lodz University of Technology, Lodz, Poland
2021	Fourth Quarter – Outstanding Research Award, Lodz University of Technology, Lodz, Poland
2020	Award from the director for Best Research Team, Institute of Fundamental Technological Research PAS, Warsaw, Poland
2020	Award from the director for Outstanding Research, Institute of Fundamental Technological Research PAS, Warsaw, Poland
2017	First Prize for Outstanding Young Research Talk, University of Cincinnati, USA

C. Contribution to Science

1. In collaboration with SMFS, we have unveiled the molecular basis of the enhanced binding mechanism present in SARS-CoV-2 variants which is employed by its receptor binding domain (RBD) to attach onto entry ACE2 receptor. Our results were published in a prestigious journal and it has been communicated in the polish and international press media (https://t.ly/eoh5). I have also supervised a multinational team (i.e. USA, Germany, Slovenia, Mexico and Poland) and together we discovered the gained mechanostability in SARS-CoV-2 RBD that has made the virion more stable and facilitating the spreading of the COVID-19 disease. It has been the first *in silico* study to report about the RBD mechanostabiity and already validated by experiments using AFM/magnetic tweezers. Also, one of our earlier publications in COVID-19 has reached >300 citation. I served as the primary investigator in all of these studies.

    a. Koehler, M., Ray, A., Moreira, R. A., Juniku, B., Poma, A. B., & Alsteens, D. (2021). Molecular insights into receptor binding energetics and neutralization of SARS-CoV-2 variants. *Nature communications*, **12**(1), 6977.
    b. Moreira, R. A., Guzman, H. V., Boopathi, S., Baker, J. L., & Poma, A. B. (2020). Characterization of structural and energetic differences between conformations of the SARS-CoV-2 spike protein. *Materials*, 13(23), 5362.
    c. Moreira, R. A., Chwastyk, M., Baker, J. L., Guzman, H. V.,& Poma, A. B. (2020). Quantitative determination of mechanical stability in the novel coronavirus spike protein. *Nanoscale*, **12**(31), 16409–16413.
    d. Boopathi, S., Poma, A. B., & Kolandaivel, P. (2021). Novel 2019 coronavirus structure, mechanism of action, antiviral drug promises and rule out against its treatment. *Journal of Biomolecular Structure and Dynamics*, 39(9), 3409-3418.

2. Furthermore, I am the main developer of the GōMARTINI approach for the sampling of large conformational changes in proteins and their complexes under the MARTINI 3 force field (http://cgmartini.nl). My original work in combining the popular MARTINI force field with a structure-based model has become a reference approach in the latest version of MARTINI 3 for biological applications where large structural changes are required. In particular, during denaturation/folding of proteins, allosteric changes due to single point mutation

that induces structural modifications, etc. The GōMARTINI approach has become a very practical tool for the study of deformation profiles of large biomolecular systems. I served as the primary investigator or co-investigator in all of these studies.

a. Poma, A. B., Cieplak, M., & Theodorakis, P. E. (2017). Combining the MARTINI and structure-based coarse-grained approaches for the molecular dynamics studies of conformational transitions in proteins. *Journal of Chemical Theory and Computation*, 13(3), 1366-1374.
b. Mahmood, M. I., Poma, A. B., & Okazaki, K. I. (2021). Optimizing Gō-MARTINI coarse-grained model for F-BAR protein on lipid membrane. *Frontiers in molecular biosciences*, 8, 619381.
c. Poma, A. B., Li, M. S., Theodorakis, P. E. (2018). Generalization of the elastic network model for the study of large conformational changes in biomolecules. *Physical Chemistry Chemical Physics*, 20(25), 17020-17028.
d. Liu, Z., Moreira, R. A., Dujmović, A., Liu, H., Yang, B., Poma, A. B., & Nash, M. A. (2021). Mapping mechanostable pulling geometries of a therapeutic anticalin/CTLA-4 protein complex. *Nano letters*, 22(1), 179-187.

3. I have participated in the development of a multiscale approach that includes quantum-classical coupling of special interest in classical simulation where quantum effects in light-mass particles (e.g. H atoms) are necessary to be described. One of these publications lead us to a Physical Review Letter (editor's suggestion). My work has profound implications at the interface between chemistry, physics and biology fields where quantum effects are still relevant. For instance, in the design of novel enzymes and correct sampling of structural properties in solvents. I served as the co-investigator in all of these studies

a. Poma, A. B., & Delle Site, L. (2010). Classical to path-integral adaptive resolution in molecular simulation: towards a smooth quantum-classical coupling. *Physical review letters*, 104(25), 250201.
b. Poma, A. B., Delle Site, L. (2011). Adaptive resolution simulation of liquid para-hydrogen: testing the robustness of the quantum-classical adaptive coupling. *Physical Chemistry Chemical Physics*, 13(22), 10510-10519.
c. Poma, A., Monteferrante, M., Bonella, S., & Ciccotti, G. (2012). The quantum free energy barrier for hydrogen vacancy diffusion in Na_3AlH_6. *Physical Chemistry Chemical Physics*, 14(44), 15458-15463.

Complete List of Published Work in MyBibliography:

https://www.ncbi.nlm.nih.gov/myncbi/adolfo.poma.1/bibliography/public/

D. Research Support

Ongoing Research Support

NCN, Nr. 2022/45/B/NZ1/02519 Adolfo Poma (PI) 01/03/2023–01/03/2026
Molecular biomechanics of SARS-CoV-2 variants: virus-host cell binding and immune evasion
The goal of this study is to characterize the nanomechanics of the full-length SARS-CoV-2 spike protein, in complex with ACE2 and with antibodies by molecular simulation.
Role: PI

NCN, Nr. 2017/26/D/NZ1/00466 Adolfo Poma (PI) 04/20/2018–04/19/2022
Self-assembly and nanomechanical characterization of cellulose microfibers
The goal of this study was to characterise the nanomechanics of cellulose assemblies by MD simulation.
Role: PI

PL-GRID, Center for High Performance Computing Adolfo Poma (PI) 07/01/2021–07/01/2022
The goal is to boost via large scale computing the study of biomolecular complexes with biomedical applications. An extension for additional year after successful completion is expected.
Role: PI