

# FRANCESCO TAVANTI



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24 august 1986, Italian

**Executive Summary:** Versatile and passionate post-doc with experience in molecular dynamics simulations of proteins and gold nanoparticles using atomistic and coarse-grained models.

papers published: 12

h-index: 4

citations: 64

source: [WebOfScience](#)

## ACADEMIC EXPERIENCE

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01/01/2017-now post-doc in the group of Prof. Menziani M. C.

University of Modena and Reggio Emilia, Modena (Italy),

<http://personale.unimore.it/rubrica/dettaglio/ftavanti>

Amyloid-beta fibrils involved in the Alzheimer's disease and fibrillation inhibitors drugs using molecular dynamics simulations

2014-2016 PhD student in Models and Methods for Material and Environmental Sciences

University of Modena and Reggio Emilia, Modena (Italy), <http://www.unimore.it>

Gold nanoparticles-proteins interaction using molecular dynamics simulations and multi-scale models.

02/06/2015- Visiting student at Massachusetts Institute of Technology

01/11/2015 Department of Materials Sciences and Engineering, MIT, <https://dmse.mit.edu>  
Gold nanoparticles-proteins interaction using molecular dynamics simulations

2009-2013 Master's degree in Medical Physics

Score: 107/110

University of Pisa, Pisa (Italy), <http://www.unipi.it>

Main subjects: ionizing radiations, magnetic fields, radiation sources, data collection and analysis, detectors for radiations, biophysics, image analysis and image reconstruction, equipment of medical interest.

## PUBLISHED PAPERS

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1. G. Ortega, **F. Tavanti**, Z. Bednarikova, Z. Gazova, G. Rigillo, C. Imbriano, V. Basile, M. Asti, L. Rigamonti, M. Saladini, E. Ferrari, M. C. Menziani. Curcumin derivatives and A $\beta$ -fibrillar aggregates: An interaction's study for diagnostic/therapeutic purpose in neurodegenerative diseases. *Bioorg. Med. Chem.* 2018, **26**, 4288-4300.
2. **F. Tavanti**, A. Pedone, M. C. Menziani. Computational Insight into the Effect of Natural Compounds on the Destabilization of Preformed Amyloid- $\beta$ (1-40) Fibrils. *Molecules*, 2018, **23**, 1320.
3. A. Pedone, **F. Tavanti**, G. Malavasi, M. C. Menziani. An atomic-level look at the structure-property relationship of cerium-doped glasses using classical molecular dynamics. *J. Non-Cryst. Sol.*, 2018, doi.org/10.1016/j.jnoncrysol.2018.03.040.
4. **F. Tavanti**, F. Muniz-Miranda, A. Pedone. The Effect of Alkaline Cations on the Intercalation of Carbon Dioxide in Sepiolite Minerals: A Molecular Dynamics Investigation. *Front. Mater.* 2018, **5**, 12.
5. D. Malferrari, F. Bernini, **F. Tavanti**, L. Tuccio, A. Pedone. Experimental and Molecular Dynamics Investigation Proves That Montmorillonite Traps the Biogenic Amines Histamine and Tyramine. *J. Phys. Chem. C*, 2017, **121**, 27493-27503.
6. **F. Tavanti**, A. Pedone, P. Matteini, M. C. Menziani, "Computational Insight into the Interaction of Cytochrome c with Wet and PVP-Coated Ag Surfaces", *J. Phys. Chem. B*, 2017, **121**, 9532-9540.
7. S. Deyev, G. Proshkina, A. Ryabova, **F. Tavanti**, M. C. Menziani, G. Eidelstein, G. Avishai, A. B Kotlyar, "Synthesis, Characterization and Selective Delivery of DARP-in Gold Nanoparticles Conjugates to Cancer Cells", *Bioconjugate Chemistry*, 2017, **28**, 2569-2574.
8. P. Matteini ,M. Cottat, **F. Tavanti**, E. Panfilova, M. Scuderi, G. Nicotra, M. C. Menziani, N. Khlebtsov, M. de Angelis, R. Pini, "Site-selective surface-enhanced Raman detection of proteins", *ACS nano*, 2017, **11**, 918-926.
9. F. Muniz-Miranda, F. Lodesani, **F. Tavanti**, D. Presti, D. Malferrari, A. Pedone, "Supercritical CO<sub>2</sub> Confined in Palygorskite and Sepiolite minerals: A Classical Molecular Dynamics Investigation", *J. Phys. Chem. C*, 2016, **120**, 26945-26954.

10. **F. Tavanti**, A. Pedone, M. C. Menziani, "Competitive Binding of Proteins to Gold Nanoparticles disclosed by Molecular Dynamics Simulations", *J. Phys. Chem. C*, 2015, **119**, 22172-22180.
11. **F. Tavanti**, A. Pedone, M. C. Menziani, "A closer look into the ubiquitin corona on gold nanoparticles by computational studies", *New J. Chem.*, 2015, **39**, 2474-2482.
12. **F. Tavanti**, V. Tozzini, "A Multi-Scale--Multi-Stable model for the Rhodopsin Photocycle", *Molecules*, 2014, **19**, 14961-14978.

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#### GRANTS

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1. **FAR2018-Junior** "Computer-aided Rational Design of Functionalized Gold Nanoparticles as Inhibitors of Amyloid- $\beta$  Oligomerization for Alzheimer's Disease Treatment". Research project for a young post-doc at the University of Modena and Reggio Emilia, 32K€, PI.

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#### TALKS

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1. **Tavanti, F.**, Ferrari E., Pedone, A., Menziani, M. C. "Computational Study of Curcumin-derivatives for Alzheimer's Disease Treatment", Italian Chemical Society, Paestum (Sa), Italy, September 10-14 2017.
2. **Tavanti, F.**, Pedone, A., Menziani, M. C. "*Specific Interactions of Gold Nanoparticles with Amyloid- $\beta$  fibrils*". Italian Chemical Society, DCTC 2015, Rome, Italy, December 14-16, 2015.
3. **Tavanti, F.**, Pedone, A., Menziani, M. C. "*Monolayer-protected Gold Nanoparticles interacting with Amyloid- $\beta$  fibrils: a Computational Study*". Giornata della Chimica dell'Emilia Romagna, Modena, Italy, December 18, 2015.

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#### PRIZES

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1. **One of the best 10** articles published by a young chemist in Italy in 2017 (Premio Primo Levi 2017 della Società di Chimica Italiana)
2. **Winner** of "Present your research in 150 seconds" from ChemPubSoc Europe and Young group of the Austrian Chemistry Association.

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#### JOURNAL'S COVER

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1. **Tavanti, F.**, Bioconjugate Chemistry, vol. 28, issue 10, 2017.

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#### POSTERS & ATTENDED SCHOOLS

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1. Winter Modeling 2014 (13/04/2014 - 14/04/2014) Modena (IT) with title: 'Computational Modeling of Protein-Nanoparticle Interactions'.

2. CCP5 Summer School in Molecular Modelling (13/07/2014 – 22/07/2014) Manchester (UK) with title: 'Computational Modeling of Ubiquitin-Corona Formation on Gold Nanoparticles'.
3. Giornata della chimica dell'Emilia Romagna (18/12/2014) Parma (IT) with title: 'Ubiquitins on gold nanoparticles: a molecular dynamics simulation'.
4. Multiscale Modelling of Condensed Phase and Biological Systems (13/04/2016 – 15/04/2016) Manchester (UK) with title: 'Monolayer-protected Gold Nanoparticles interacting with Amyloid Fibrils'.
5. Italian Chemical Society 2017 (10/09/2017 – 14/09/2017), Paestum (IT) with title: 'Molecular Dynamics Simulations of Amyloid-beta fibrils for Alzheimer's Theranostic Applications'
6. Italian Chemical Society, DCTC2018 (19/09/2018 – 21/09/2018), Trieste (IT) with title: 'Natural compounds for Alzheimer's disease treatment: a classical Molecular Dynamics investigation'
  - I. CCP5 Summer School in Molecular Modelling: 'Methods in molecular simulations' (13/07/2014 – 22/07/2014) Manchester (UK). Advanced course in 'Meso-scale Methods'.

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### PROJECTS for accessing High Performance Computing resources

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1. ISCRA-C grant (2015): Proteins corona formation on gold nanoparticles, Galileo@CINECA (Tier 1), 75Khrs; PI
2. ISCRA-C grant (2016): Gold nanoparticles interacting with Alzheimer's fibrils, Galileo@CINECA (Tier 1), 35Khrs; PI
3. PRACE – Preparatory Access (2016): Insight into Silver Nanocube-protein interaction by computational simulations, Fermi@CINECA (Tier 0), 100Khrs; MareNostrum@BSC-CNS (Tier 0), 50Khrs; coll.
4. ISCRA-C grant (2017): Curcumin-like compounds for Amyloid Inhibition, Marconi@CINECA (Tier 1); 26Khrs, PI.

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### TEACHING

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2016 and 2017 "Hands on" computational exercises for the course "Chimica computazionale" held by Prof. Menziani M. C.. Corso di Laurea Magistrale in Chimica, Università di Modena e Reggio Emilia.

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### REFERRING ACTIVITY

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Since 2016, I've been assigned review duty by *RSC Advances*, *MDPI International Journal of Molecular Sciences*, *MDPI Materials*, *Journal of Molecular Liquids*.

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### SKILLS

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Languages: Italian (mother tongue), English: TOEFL iBT exam with score 90/120 and PET, good working knowledge.

Computer: Expertise on Windows and Mac OS, Office, Fortran, Matlab, DL\_POLY, Gromacs, VMD, AutoDock, Gnuplot, GDIS, UCSF Chimera, Jmol and Swiss PDB Viewer. Knowledge of DL\_MESO, DL\_FIELD and Material Studio.

## REFERENCES

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Maria Cristina Menziani, Professor of Chemistry at the University of Modena and Reggio Emilia, [mariacristina.menziani@unimore.it](mailto:mariacristina.menziani@unimore.it)

Alfonso Pedone, Professor of Chemistry at the University of Modena and Reggio Emilia, [alfonso.pedone@unimore.it](mailto:alfonso.pedone@unimore.it)

Valentina Tozzini, Scientist at the NEST-CNR-Nanoscience Institute at Scuola Normale Superiore, Pisa, [v.tozzini@sns.it](mailto:v.tozzini@sns.it)

Alfredo Alexander-Katz, Walter Henry Gale Associate Professor at Massachusetts Institute of Technology, Cambridge, MA, [aalexand@mit.edu](mailto:aalexand@mit.edu)

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