Mahdi Tavakol, BSc, MSc, PhD.

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QUALIFICATIONS SUMMARY

- Result-oriented individual with superb collaborative and technical communication skills offering a deep understanding of molecular simulation of various systems obtained through 12 years of experience.
- Demonstrated high standard of research output through publishing peer reviewed papers in internationally acclaimed journals including "Nature Scientific Reports" and "ACS Nano" with total citation of 254 and h-index of 7.
- Experience in molecular simulation of proteins (All-Atom and Coarse-Grained MD).
- Experience in the use of High Performance Computing systems (HPC) of: Summit, ICHEC, BEDE, Hamilton, Archer2, ARC, Bluebear.
- Successful in securing two highly competitive travel grants.
- Extensive hands-on experience with LAMMPS, NAMD, GROMACS, VMD and OVITO molecular simulation/visualization packages.
- Understanding of the LAMMPS source code and experience in adding new commands to the software package.
- Good experience in programming in C++ and Python and familiarity with CUDA C, bash, MATLAB and tcl scripting languages.
- Familiarity with Gaussian.
- Proficient in Linux OS.
- Time management skills.
- B.Sc, M.Sc. and Ph.D. degrees from 1st ranked Iranian university.

RESEARCH AND TECHNICAL SKILLS

- **Molecular Dynamics simulations**: Conventional MD algorithms, Free energy methods of Jarzynski, Umbrella Sampling, Metadynamics. All-Atom simulations forcefields of CHARMM, Embedded Atom Method and Interface forcefields. Coarse grained molecular simulation forcefield of Martini. MD packages of LAMMPS, Gromacs, NAMD, VMD. **Molecular Docking:** HADDOCK.
- **Programming:** C++ (Dynamic memory allocation, pointers, operator overloading, class inheritance, understanding of object-oriented programming in C++), MATLAB, CUDA C, Bash scripting, Tcl scripting, MPI in C.
  Python: Matplotlib, Pandas, Sklearn, Numpy, XGBoost.
- **Experience in writing pipelines for automation and analysis of simulation results in:** C++ and bash shell.
- **Debugging:** GDB
- **Machine Learning:** Random Forests, K-Nearest Neighbors, Neural Networks.
- **Tools:** MS Excel, MS Word, MS PowerPoint, MS Visual Studio 2022, Endnote X20, Libreoffice Calc, Origin. Slurm HPC**.**
- **Research:** Formal training in quantitative and qualitative research methods during M.Sc. and Ph.D. educations.

PROFESSIONAL EXPERIENCE

Postdoctoral Researcher, University of Oxford, Oxford, England, UK **2024 – Present**

Department of Engineering Science

- Studying the tooth mineralization through molecular dynamics and link the results with experimental observations.
- Calculation of the hydroxyapatite dissociation through application of the Jarzynski equation to the SMD simulations
- Applying thermodynamics integration (FEP) to quantify the chemical stability.
- Writing a metadynamics command for the LAMMPS software (Object oriented programming and class inheritance concepts).

Postdoctoral Researcher, University of Durham, Durham, England, UK **2022 – 2024**

Department of Physics

- Studied the electric double layer near silica and lipid bilayer surfaces through molecular dynamics.
- Linked experimental results with molecular dynamics simulation outcomes.
- Implemented the AC field in the LAMMPS molecular dynamics software package.
- Developed several bash and python codes to automate the analysis of the simulation trajectories.
- Prepared and presented written and verbal communications.

Visiting Scholar, University of Colorado at boulder, Boulder, CO, USA **2017 – 2018**

Department of Chemical and Biological Engineering **2022 – 2023**

- Pioneered the first MD protocol to study the role of proteins in bone remodeling.
- Discovered the role of osteocalcin (protein) in bone mineralization for the first time.
- Developed in-house C++ software to analyze the Jarzynski free energy calculation outcome.

Postdoctoral Researcher, National University of Ireland, Galway, Galway, Ireland **2019 – 2022**

Biomedical Engineering and Biomechanics Research Center

- Co-supervising PhD students.
- Discovered the role of non-collagenous proteins in bone strength and the effect of protein glycation on this role.
- Discovered the effect of extrafibrillar mineralisation on the bone behavior.
- Achieved 50% higher efficiency in processing MD output data through bash scripting.
- Developed in-house python codes to build the coarse-grained model of collagen.
- Prepared and presented written and verbal communications.
- Delivered lectures on the effect of protein glycation on the bone behavior during diabetes in well recognized national and international conferences.

HONORS

- In National University Entrance Exams for B.Sc. M.Sc. and Ph.D in years 2008, 2012, 2014 ranked ***402nd , 2nd and 1st*** **among more than 319000, 25000 and 1000** candidates, respectively.
- In National Student Olympiad in 2012 ranked 17th, Iranian National Elite Foundation prizes in 2016 and 2017, Iranian National Elite Sabbatical Scholarship in 2018.

RESEARCH EXPERIENCE

- Molecular Dynamics Simulation of proteins, polymers and nanoparticles (Extensive Experience, been using MD from 2012).
- Amyloid aggregation in Type-2 diabetes.
- Stress wave consolidation of nano-composites.
- The practice of personalized medicine for drug delivery applications.
- Hydroxyapatite – protein interactions.
- Molecular Dynamics of solid-liquid interfaces.

CERTIFICATES And COURSES

- **C++ (Intermediate):** Certificate from Hackerrank, **Problem Solving (Intermediate):** Certificate from Hackerrank, **Python:** Certificate from Kaggle, **Intro to machine learning**: Certificate from Kaggle, **Intermediate machine learning:** Certificate from Kaggle, **Feature Engineering:** Certificate from Kaggle, **Data Cleaning:** Certificate from Kaggle, **Intro to Deep Learning:** Certificate from Kaggle. Attended "**Debugging, Testing and Correctness Workshop**" held by Department of Computer Science of Durham University. Attended "**Message-passing programming with MPI**", "**Advanced Message-Passing Programming**" and "**Shared Memory Programming with OpenMP**" held by Edinburgh Parallel Computing Center (EPCC). Attended "**ONETEP Masterclass**" held at Rutherford Appleton National Laboratory.

INTERNATIONAL COLLABORATIONS

- Collaboration with researchers from University of Western Australia, Sorbonne Universite and University of Sydney on the "Amorphous Solid formation at the Solid/Liquid Interfaces".
- Collaboration with researchers from Sloan Kettering Institute for Cancer Research of New York, Sapienza University of Rome and Harvard school of medicine on the "Personalized Medicine Concept".
- Collaboration with researchers from Aarhus University, Freie University, Karolinska Institutet, Tehran University of Medical sciences and Harvard school of medicine on the "Nanoparticle therapy for the Parkinson's disease".

PUBLICATIONS

- **M. Tavakol*,** T.J. Vaughan. 'Elucidating the role of diverse mineralisation paradigms on bone biomechanics - a coarse-grained molecular dynamics investigation', Nanoscale 2024.
- **M. Tavakol,** S.E Hoff, J. Liu and H. Heinz, 'Osteocalcin: Promoter or Inhibitor of the HAp Growth?', Langmuir 2024.
- J. Wang, H. Li, **M. Tavakol**, A. Serva, B. Nener, G. Parish, M. Salanne, G. Warr, K. Voïtchovsky, R. Atkin. 'Ion Adsorbed at Amorphous Solid/Solution Interfaces in Wigner Crystal-Like Structures', ACS Nano, 2024.
- W. Trewby, **M. Tavakol,** K. Voïtchovsky. 'Towards local tracking of dissolved ions at solid-liquid interfaces'. Invited review in Materials Today Physics 2024.
- **M. Tavakol*,** T.J. Vaughan. 'The effect of mineral arrangement on the mechanical properties of mineralised collagen fibrils', Journal of Royal Society Interface, 2023.
- F. Beyranvand, A. Khosravi, F. Zabihi, M. Nemati, M.F. Gholami, **M. Tavakol**, S. Beyranvand, S. Satari, J. Rabe, A. Salimi, C. Cheng, M. Adeli. 'Synthesis of Chiral Triazine Frameworks for Enantiodiscrimination', ACS Applied Material Interfaces, 2023.
- **M. Tavakol,** M.J. Hajipour, M. Ferdousi, S. Zanganeh, L. Maurizi. 'Competition of opsonins and dysopsonins on the nanoparticle surface', Nanoscale, 2023.
- **M. Tavakol,** T.J. Vaughan. 'Energy dissipation of osteopontin at a HAp mineral interface: Implications for bone biomechanics', Biophysical Journal, 2022.
- **M. Tavakol,** T.J. Vaughan. 'The role of the osteocalcin-osteopontin protein complex in bone biomechanics: a key contributor to energy dissipation at mineral-mineral interfaces', Biophysical Journal 2022.
- **M. Tavakol,** T.J. Vaughan. 'The structural role of osteocalcin in bone biomechanics and its alteration in Type-2 Diabetes', Scientific Reports, 2020.
- **M. Tavakol,** A. Montazeri, S.H Aboutalebi, R. Asgari, 'Mechanical Properties of Graphene Oxide: The Impact of Functional Groups', Applied Surface Science, 2020.
- H. Mohammad-Beigi , N. Hosseini , M. Adeli , M.R. Ejtehadi , G. Christiansen , C. Sahin , Z. Tu , **M. Tavakol ,** A. Dilmaghani-Marand , I. Nabipour , F. Farzadfar , D. Otzen , M. Hajipour and M. Mahmoudi**,** 'Mechanistic Understanding of the Interactions of Nanoparticles and α-synuclein', ACS Nano, 2019.
- **M. Tavakol**, A. Montazeri, R. Naghdabadi, M.J. Hajipour, S. Zanganeh, G. Caracciolo and M. Mahmoudi**,** 'Disease-related metabolites affect protein–nanoparticle interactions', Nanoscale, 2018.

- **M. Tavakol**, M. Mahnama, and R. Naghdabadi, 'Shock Wave Sintering of Al/SiC Metal Matrix Nanocomposites: A Molecular Dynamics Study', Computational materials science, 2016.
- **M. Tavakol**, M. Mahnama, and R. Naghdabadi, 'Mechanisms governing microstructural evolution during consolidation of nanoparticles', Materials and manufacturing processes, 2015.
- **M. Tavakol*,** K. Voïtchovsky. **'**Water and ions in electrified silica nano-gaps: a molecular dynamics study', Under review by Physical Chemistry Chemical Physics.
- **M. Tavakol*,** T.J. Vaughan. **'**Radial distribution of minerals in the mineralised collagen fibrils: A coarse grained molecular dynamics study', Manuscript prepared.
- **M. Tavakol*,** T.J. Vaughan. **'**The interplay of length and mineral content on the load response of mineralised collagen fibrils', Manuscript prepared.
- W. Trewby, **M. Tavakol,** K. Voïtchovsky. 'Direct local measurements of lipid membrane diffusion through AFM nano-rheology'. In preparation.

PRESENTATIONS AT CONFERENCES

- **M. Tavakol,** K. Voïtchovsky. 'Electrified Nano-Gaps Under AC Field: A Molecular Dynamics Study', 245th Electrochemical Society Meeting, San Fransisco, California, 2024.
- **M. Tavakol,** T.J. Vaughan. 'A Steered Molecular Dynamics Investigation on the Role of Glycation on the Energy Dissipation Capacity of Osteopontin at Mineral Interfaces in Bone', 67th Biophysical Society Annual Meeting, San Diego, California, 2023.
- **M. Tavakol,** T.J. Vaughan. 'The Effect of Mineral Distribution on the Deformation Mechanisms of Mineralised Collagen Fibrils', 11th European Solid Mechanics Conference, Galway, Ireland, 2022.
- **M. Tavakol,** T.J. Vaughan. 'A Coarse Grained Model of Mineralised Collagen Fibril Biomechanics: Understanding the Role of Extrafibrillar Mineralization', 27th Congress of European Society of Biomechanics, Porto, Portugal, 2022.
- **M. Tavakol,** T.J. Vaughan. 'A Molecular Dynamics Investigation of the Mechanical Properties of Mineralized Collagen Fibrils: the Role of Mineral Distribution', 9th World Congress of Biomechanics, Taipei, Taiwan, 2022.
- **M. Tavakol,** T.J. Vaughan. 'Energy Dissipation Mechanisms of Non-Collagenous Proteins at Mineral Interfaces in Bone'. XVI International Conference on Computational Plasticity. Fundamentals and Applications (COMPLAS 2021), Barcelona, Spain, 2021.
- **M. Tavakol,** T.J. Vaughan. 'A Molecular dynamics investigation into the structural role of non-collagenous proteins in bone biomechanics', 26th Congress of European Society of Biomechanics, Milan, Italy, 2021.
- **M. Tavakol,** T.J. Vaughan. 'Osteocalcin: A Small Protein, A Big Role In Bone Biomechanics', 26th Bioengineering in Ireland Conference, Carlow, Ireland, 2020.
- **M. Tavakol,** S.E. Hoff, J. Liu and H. Heinz, 'Mechanism of osteocalcin interactions with hydroxyapatite surfaces and hydrogen phosphate precursors for bone mineralization'. 256th ACS National Meeting & Exposition, Boston, Massachusetts, USA. 2018.
- **M. Tavakol,** M. Dehghany Dahaj, R. Naghdabadi, 'Visco-elastic behavior of microtubules: A coarse grained molecular dynamics study'. 6th International Conference on Nanostructures, Kish Island, Iran. 2016.
- **M. Tavakol. M. Mahnama, and R. Naghdabadi,** 'Shock Wave Sintering of Metal Matrix Nano-composites'. 24th International Conference on Mechanical Engineering, Yazd, Iran. 2016.
- **M. Tavakol,** and R. Naghdabadi**,** 'Activation Energy for Sintering of Nickel Nanoparticles: A Molecular Dynamics Study', 5th International Conference on Nanostructures, Kish Island, Iran. 2014.
- **M. Tavakol,** M. Mahnama, and R. Naghdabadi, 'Temperature effect on the sintering of nickel nanoparticles: A molecular dynamics study', 5th International Congress on Nanoscience & Nanotechnology, Tehran, Iran. 22-24 October 2014.

RELATED PROFESSIONAL EXPERIENCE

- Delivering an invited presentation in the 11th European Solid Mechanics Conference. Galway, Ireland, 2022.
- Chairing a session in the 11th European Solid Mechanics Conference. Galway, Ireland, 2022.
- Research assistant in the Sharif University.
- Reviewing papers in Science Progress, Computer Methods in Biomechanics and Biomedical Engineering journals.
- Teaching in Durham University.

TEACHING AND MENTORING EXPERIENCES

- Managing a team of three Master students in Sharif University.
- Teaching assistant for four courses in Sharif University.
- Teaching assistant for two courses in Durham University.

EDUCATION

PhD in mechanical engineering, Sharif University of Technology, Iran	**2018**
MSc in mechanical engineering, Sharif University of Technology, Iran	**2014**
BSc in mechanical engineering, Isfahan University of Technology, Iran	**2012**