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Career Progression

April 2024 – present — **Specially Appointed Researcher**, WPI Premium Research Institute for Human Metaverse Medicine (WPI-PRIMe), Osaka University, Osaka, Japan.

April 2023 – March 2024 — **Lecturer**
Physics Department, Faculty of Science, Ain Shams University, Cairo, Egypt.

April 2022 – March 2023 — **Postdoctoral researcher, Molecular Modeling and Simulation (MMS) Team**, National Institute for Quantum Science and Technology (QST), Chiba, Japan.

Dec. 2016 – April 2019 — **Senior Teaching/Research Assistant**
Physics Department, Faculty of Science, Ain Shams University, Cairo, Egypt.

March 2010 – Dec. 2016 — **Junior Teaching/Research Assistant**
Physics Department, Faculty of Science, Ain Shams University, Cairo, Egypt.

Education

April 2019 – March 2022 — **Ph.D., School of Life Science and Technology, Tokyo Institute of Technology** in Computational Biology.
Thesis title: *Investigating Dissociation Process and Binding Free Energy of P53-DBD/DNA Complex by PaCS-MD and MSM.*

June 2012 – October 2016 — **M.Sc., Faculty of Science, Ain Shams University** in Biophysics.
Thesis title: *Genetic and Physiological Effects of Ultraviolet Radiation on Tomato Plant (solanum lycopersicum).*

September 2005 – June 2009 — **B.Sc., Faculty of Science, Ain Shams University** in Biophysics.

Research Publications

Journal Articles

1. Sobeh, M. M., & Kitao, A. (2022). Dissociation pathways of the p53 DNA binding domain from DNA and critical roles of key residues elucidated by dPaCS-MD/MSM. *Journal of Chemical Information and Modeling*, *62*(5), 1294–1307. doi:10.1021/acs.jcim.1c01508

2. Hata, H., Tran, D. P., Sobeh, M. M., & Kitao, A. (2021). Binding free energy of protein/ligand complexes calculated using dissociation parallel cascade selection molecular dynamics and markov state model. *Biophysics and Physicobiology*, *18*(0), 305–316. doi:10.2142/biophysico.bppb-v18.037

Conference Proceedings

1. Sobeh, M. M., Kono, H., & Sakuraba, S. (2023.2.18). Predicting the Salt Bridges Contribution to Protein Stability using the Free-Energy Perturbation and Enhanced Sampling Approach. In *Proceedings of the 67th Annual Meeting of the Biophysical Society*, Poster, San Diego, California, US.

2. Sobeh, M. M. (2021.9.16). Investigating the dissociation process and binding free energy of the p53-DBD/DNA complex by PaCS-MD and MSM. In *Proceedings of The Third International Online Conference on Molecular Modeling and Spectroscopy*, Short presentation, Online Conference, Giza, Egypt. Retrieved from https://www.youtube.com/watch?v=wroOofDsxos

3. Sobeh, M. M., & Kitao, A. (2021.4.28). Investigating the dissociation process and binding energy of the p53-DBD/DNA complex by PaCS-MD and MSM. In *Proceedings of WE-Heraeus-Seminar, Advanced Physical and Computational Techniques to Investigate Protein Dynamics*, Poster, Online Conference via MeetAnyway, Freie Universität Berlin, Germany. Retrieved from https://shortest.link/2mnF

4. Sobeh, M. M., & Kitao, A. (2021.6.16). Investigating the dissociation process and binding free energy of the p53-DBD/DNA complex by PaCS-MD and MSM. In *Proceedings of the 21st Annual Meeting of the Protein Science Society of Japan*, Poster, Online Conference, Tokyo, Japan.

Invited Talks / Presentations

Feb., 2025 — **Accelerating Biomolecular Simulations with Enhanced Sampling Techniques**. 2nd Serial Networking of Foreign Researchers: Sysmex - Osaka University, Osaka, Japan.(**10-minute Presentation**)

Grants

March, 2023 — **Early-Career Scientists, KAKENHI, Japan**, (**Principal Investigator**). Molecular Dynamics Simulation for Association/Dissociation of Protein-Ligand and Protein-DNA Complexes by Advanced Enhanced Sampling Technique, **3 years** (**5 000 000 Yen**.)

Research Skills

MD Simulation	Molecular dynamics (MD) simulations for protein-DNA, Protein-Protein complexes.
Enhanced sampling MD	Enhanced sampling MD simulations using techniques such as using PaCS-MD, REMD, gREST, and REUS.
Binding Free energy	Binding Free energy predictions using MSM, FEP, and MMBPSA.
Protein predictions	Protein and peptide structure predictions using Modeller, SWISS-MODEL, and AlphaFold.

Other Skills

Languages	English: strong reading, writing, and speaking. Japanese: basic reading, writing, and speaking (JLPT N5).
Coding	Python, Bash scripting, Tcl, C++, LaTeX, Git.
MD Packages	AMBER, GROMACS, GENESIS, Autodock vina, Rosetta, PyRosetta, Modeller.
MD Analysis	VMD, PyMOL, ChimeraX, PLIP, PyEMMA, Mdtraj, MDAnalysis.
Machine Learning	SciKit Learn, TensorFlow, Keras, PyTorch.
Cheminformatics	RDKit.

Miscellaneous Experience

Awards and Achievements

2021 – 2022 **Cross the border**, Tokyo-Tech pioneering doctoral research program by Tokyo Institute of Technology.

2019 – 2021 **Tokyo Tech Tsubame Scholarship**, Tokyo Institute of Technology.

Ph.D. Scholarship, The Egypt-Japan Education Partnership (EJEP).

2010 **Medal of Superiority**, Faculty of Science, Ain Shams University, Cairo, Egypt.

Workshops, Training and Online Courses

June, 2024 **IUPAB 2024 Hands-on Training Program**, CHARMM-GUI/GENESIS MD Tutorial, RIKEN, Kobe, Japan.

January, 2024 **Deep Learning Specialization**, Stanford ONLINE & DeepLearning.AI, Coursera Platform (Prof. Andrew Ng).

November, 2023 **Machine Learning Specialization**, Stanford ONLINE & DeepLearning.AI, Coursera Platform (Prof. Andrew Ng).

February, 2022 **Fundamentals of Deep Learning**, NVIDIA Deep Learning Institute.

June, 2021 **BioExcel Summer School on Biomolecular Simulations**, Centre of Excellence for Computational Biomolecular Research.

March, 2021 **Introduction to Simulation Environments for Life Sciences**, Online PATC@BSC Training Course.