

Education

- Development of autonomous propulsion mechanisms for the rotary motor.
- Development of DNA origami structures and tools for the purpose of artificial molecular machines.

- **B.Sc. in Chemical Engineering:** Completed a senior year project involving the design of a butyl alcohol production plant.
- **B.Sc. in Chemistry:** Specialized in physical chemistry, conducted research on project on DNA origami dimerization yield.

Research and Work Experience

Developing a functioning autonomous artificial molecular motor with all the key properties of the biological one is an unprecedented achievement. In this project, I introduced a concept and validated it through computer kinetics simulations. Key highlights include:

- I developed an autonomous motor mechanism that leverages our origami rotor framework, incorporating a unique symmetry-breaking method based on rotor geometry.
- Utilizing extensive knowledge of DNA reaction schemes, the developed mechanism employs a metastable DNA hairpin as fuel for the DNA bipedal walker. The walker is attached to the upper part of the rotor, allowing it to stride along footholds placed in the lower part.
- To validate and optimize various settings, I analyzed all possible interaction states and collected several DNA reactions constants. I Built a mathematical model to describe the system, and conducted time-course simulations, further employing multidimensional optimization methods to fine-tune parameters.
- Theoretical analysis revealed an impressive stepping rate of 1-3 minutes with less than 2% error per step.

- I designed a ~90nm diameter disc structure that acts as the stator. This disc can be connected via swivel to the upper disc that is free to rotate. The rotor assembly houses a circular footholds track (an 'infinite' track), a bipedal walker, and a 75x25nm gold nanorod. The nanorod is used to track the rotation via defocused light-scattering technique.
- High folding purity was achieved for the desired structure by following the standard and advanced considerations, utilizing self-developed tools, such as scaffold sequence redundancy analyzer. Additionally, I employed multiple molecular dynamic simulations methods to iteratively correct the inherent origami global twist. Cryo-TEM reconstruction confirmed our goal creating flat disc rotates without self-collisions.
- Furthermore, I contributed to the initial experimental phase, ultimately our team achieved 72 steps equivalent to 6 full turns of externally controlled walking, with 60% final yield (to be submitted to *nature communications*).

- I designed a DNA origami capsule measuring approximately 100x35nm. Other lab members are currently using this capsule to investigate foothold interactions with the base. Insights gained from this research may contribute to foothold integrity, ultimately to improving stepping yield.
- Additionally, I developed a mini origami structure measuring approximately 20x7nm, rod-shaped. This structure will be attached to a linear bipedal walker by other lab members. The attachment will introduce drag effects, which would amplify the errors and provide a means for better understanding.

D. DNA origami Dimer and Hexamer Reactions

During my senior year of bachelor's studies, I led a project focused on dimer reactions which extended into my PhD. By identifying and eliminating limiting factors, I achieved a very high yield of 99%, much higher than the typical 80% yield for such a reaction. This work was published in a *small journal*.

- Scaling the reaction to a 6-mer track (1 μ m long), presented additional challenges. I discovered that random, unintentional interactions originating from the hybridization site hindered the correct reaction due to aggregation. To address this, I developed a tool called "NuCraft". It generates a pseudo-random sequence for the hybridization site while ensuring that no unintended segment hybridization occurs beyond a user-defined order. With other technical adjustments, we achieved an impressive 90% yield for the full hexamer. The paper is in publication process for *small journal*.

E. Teaching Assistant at Ben Gurion University | 2019 – 2024

General Chemistry lab instructor for undergrads at various levels, including pharmacists, biologists, and chemists.

Skills

- **Scientific Expertise:** DNA Nanotechnology, DNA origami based nanomachines, DNA dynamics, Single molecule fluorescence and scattering and Microfluidics technology.
- **Personal Skills:** As an *observant* individual, I excel at identifying patterns and nuances, allowing me to approach problem-solving with precision. My *adaptability* enables me to thrive in dynamic environments, where I can quickly adjust to changing circumstances. Moreover, my *proactive* mindset empowers me to build cohesive and effective teamwork, fostering collaboration and achieving shared goals.
- **Computer Simulations and Analysis:** Proficient in various molecular dynamic simulations, including ENRG MD, all-atom, and mrDNA. Developed custom tools and scripts for DNA sequence analysis, as well as a unique-sequence DNA generator using *MATLAB*. Additionally, wrote *Python* scripts to find optimized solutions for multidimensional, out-of-equilibrium chemical reaction systems.
- **Software Proficiency:** Skilled in various visualization software, such as *VMD*, *Maya*, *Corel-Draw*, and *Chimera*. Experienced with image analysis tools like ImageJ and Gwydion.
- **Laboratory Skills:** Knowledgeable in optical table setups, including lasers, fibers, and cameras, as well as AFM, and TEM measurements. Competent in techniques such as Agarose Gel Electrophoresis and PEG purification, and Proficient in nucleic acid hybridization reactions.
- **Languages:** English and Hebrew (Full Professional Proficiency), Arabic (Native).

Scholarships

- "Southern Lakhish" scholarship for excellence: Awarded to direct track PhD students by Kreitman School, totaling 330K₪ over 5-years (2019-2024). Additionally, the Faculty of Natural Sciences granted a separate 5-year tuition scholarship.
- Excellence scholarship fellowship for the summer: Awarded by Faculty of Natural Sciences in 2019, 5200 ₪.

Publication

- **Sheheade, B.**, Liber, M., Popov, M., Berger, Y., Khara, D. C., Jopp, J., & Nir, E. (2019). Self-Assembly of DNA Origami Heterodimers in High Yields and Analysis of the Involved Mechanisms. *Small*, 15(51), 1902979.
- **Sheheade, B.**, Popov, M., Basak, S., Shapira, H., Khara, D. C., & Nir, E. Fabrication of a Micrometer Long DNA Hexamer Nanoribbon at High Yield and Purity – Publication process to *Small*.
- Shapira, H.; **Sheheade, B.**; Khara, D. C., Basak, S, D. C., & Nir, E. A DNA Origami Rotary Motor Operated by a Microfluidic Device and Monitored by Defocused Imaging - To be submitted to *nature communication*.