Ashim Nandi

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Professional Experience

2022- **Research Associate** University of Southern California, USA.
Advisor: Dr. Arieh Warshel (Distinguished Professor, and 2013 Chemistry Nobel Laureate).

2021-2022 **Postdoctoral Fellow** Weizmann Institute of Science, Israel.
Advisor: Dr. Jan (Gershom) Martin (Professor, and 2023 Schrödinger Medalist).

Education

2016-2021 **MS-Ph.D.** in Chemistry *(Summa cum Laude)* — Ben-Gurion University of the Negev, Israel.
Thesis: *Computational Studies of Light and Heavy Atom Quantum Tunneling in Organic Reactions*
Advisor: Professor Sebastian Kozuch

2013-2015 **M.Sc.** in Chemistry *(Gold Medalist)* — North-Eastern Hill University (NEHU), India.
Thesis: *Competition between Hydrogen and Halogen Bonding in Sulfur-based Compounds and Hypohalous Acid*
Advisor: Professor Asit K. Chandra

2010-2013 **B.Sc.** *(University Ranked 6th)* — St. Edmund's College, NEHU, India.
Major: *Chemistry*. Minor: *Physics* and *Math*.

Honors and Awards

2024 Selected as a Mars Fellow for the 73rd Lindau Nobel Laureate Meeting, Germany.
2024 Invitation as a Young Scientist to the 73rd Lindau Nobel Laureate Meeting, Germany.
2024 DST-INSPIRE Faculty Fellowship Award, Government of India, India.
2021 Dean's Excellence Postdoctoral Fellowship, Weizmann Institute of Science.
2021 University's Rector Prize for Excellence in Ph.D. (*Summa cum Laude*), Chemistry.
2017-2021 Negev-Tsin Scholarship for Ph.D., Chemistry.
2017 ADAMA Prize for Excellence in M.S. Thesis.
2015 Rector Gold Medal for M.Sc., Chemistry.
2013-2015 Oil and Natural Gas Corporation (ONGC) India Scholarship for securing the First Rank in M.Sc. Chemistry at the University.

List of Publications **May 2024**

Notes: 1) * denotes corresponding author. 2) † Equally contributed. 3) Titles in blue are clickable links.

Peer-Reviewed Publications

18. M. Asadi, A. Nandi, and A.Warshel*
Computational Mechanistic Insights into Reversible and Irreversible Covalent Inhibitors Targeting SARS-CoV-2 Mpro
Biochemistry **2024** (Submitted, *under minor revision*).

17. A. Nandi, A. Zhang, Z. T. Chu, W. Xie, Z. Xu, S. Dong, A.Warshel*
Exploring the Light-Emitting Agents in Renilla Luciferases by an Effective QM/MM Approach
Journal of the American Chemical Society **2024** (Just published) (**IF 15.0**).

16. A. Nandi†, A. Zhang†, E. Arad, R. Jelenik, and A. Warshel*
Assessing the Catalytic Role of Native Glucagon Amyloid Fibrils
ACS Catalysis **2024**, 14, 4656-4664 (**IF 12.9**).

15. W. Jun Xie†,* D. Liu†, X. Wang†, A. Zhang, Q. Wei, S. Dong, A. Nandi, and A. Warshel*
Enhancing luciferase activity and stability through generative modeling of natural enzyme sequences
Proceedings of the National Academy of Sciences **2023**, 120(48), e2312848120 (**IF 11.1**).

14. Z. Alassad†, A. Nandi†, S. Kozuch*, and A. Milo*
Reactivity and Enantioselectivity in NHC Organocatalysis Provide Evidence for the Complex Role of Modifications at the Secondary Sphere
Journal of the American Chemical Society **2023**, 145, 1, 89-98 (**IF 15.0**).

13. P. Das, A. Roy, A. Nandi, I. Neogi, Y. Posner, I. Pinkas, S. Kozuch, M. Firer, M. Montag*, F. Grynszpan*
Thioxobimanes
Journal of Organic Chemistry **2023**, 88 (19), 13475-13489 (**IF 4.5**).

12. A. Nandi*, and J. Martin*
Thermally-Activated Tunneling in the Two-Water Bridge Catalyzed Tautomerization of Phosphinylidene Compounds
ChemPhysChem **2022**, 23, e2022003 (**IF 3.52**).

11. A. Nandi*, and J. Martin*
Heavy-Atom Tunneling in the Covalent/Dative Bond Complexation of Cyclo[18]carbon–piperidine
Journal of Physical Chemistry B **2022**, 26, 1799–1804 (**IF 3.5**).

10. R. Manikandan, N. Shauloff, A. Nandi, A. Pevzner, S. Marx, R. Jelinek*
Visual Organophosphate Vapor Sensing by Dibenzylidine Derivatives Exhibiting Intramolecular Charge Transfer and Aggregation Induced Emission
Journal of Materials Chemistry C **2022**, 10, 5458-5465 (**IF 6.6**).

9. A. Nandi*, Z. Alassad, A. Milo, and S. Kozuch
Quantum Tunneling on Carbene Organocatalysis: Breslow Intermediate Formation via Water-Bridges
ACS Catalysis **2021**, 11, 14836–14841 (**IF 12.9**).

8. S. Gadekar†, V. Dhayalan†, A. Nandi, I. Zak, S. Barkai, M. Shema-Mizrachi, S. Kozuch, A. Milo*
Rerouting an Organocatalytic Reaction by Intercepting its Reactive Intermediates
ACS Catalysis **2021**, 11, 14561–14569 (**IF 12.9**).

7. A. Nandi†, N. Tarannam†, D. R. Silva, C. F. Guerra, T. A. Hamlin*, and S. Kozuch*
Boron Tunnelling in the "Weak" Bond-stretch Isomerization of N-B Lewis Adducts
ChemPhysChem **2021**, 22, 1857-1862 (**IF 3.52**).

6. A. Nandi*, S. Kozuch, and J. Kästner
Comment on "Computational evidence for sulfur atom tunneling in the ring flipping reaction of S4N4"
Chemical Physics Letters **2020**, 754, 137678 (**IF 2.8**).

5. A. Nandi, A. Sucher, A. Tyomkin, and S. Kozuch*
Ping-Pong Tunneling Reactions, Part 2: Boron and Carbon Bell-Clapper Rearrangement
Pure and Applied Chemistry **2020**, 92, 39-47 (**IF 1.8**).

4. A. Nandi, E. Solel, and S. Kozuch*
Carbon Tunneling in the Automerization of Cyclo[18]Carbon
Chemistry – A European Journal **2020**, 26, 625-628 (**IF 5.02**).

3. A. Nandi, and S. Kozuch*
History and Future of Dative Bonds
Chemistry – A European Journal **2019**, 25, 1-15 (**IF 5.02**).

2. A. Nandi[†], A. Sucher[†], and S. Kozuch*
Ping-Pong Tunneling Reactions: Can Fluoride Jump at Absolute Zero?
Chemistry – A European Journal **2018**, 24, 16348-16355 (**IF 5.02**).

1. A. Nandi, D. Gerbig, P. R. Schreiner, W. T. Borden, S. Kozuch*
Isotope-Controlled Selectivity by Quantum Tunneling: Hydrogen Migration versus Ring Expansion in Cyclopropylmethyl Carbenes
Journal of the American Chemical Society **2017**, 139, 9097-9099 (**IF 15.0**).

Book Chapters

1. A. Nandi, G. Molpeceres, P. K. Gupta, J. Martin, J. Kästner, D. T. Major, S. Kozuch*
Quantum Tunneling in Computational Catalysis and Kinetics: Is it Really Important?
Chapter in reference work Comprehensive Computational Chemistry (edited by Russell J. Boyd and Manuel Yañez), Vol. **4**, pp. 713-734 (**2024**).

Teaching Experience – Summarized

As Teaching Assistant at Ben-Gurion University

2019-2021 – *Applied Computational Chemistry*

2017-2021 – *Quantum Chemistry & Chemical Bonding*

Oral Presentations at International Conferences

4. **Next Generation Science: The 73rd Lindau Nobel Laureate Meetings**
Breaking Down the Plastic Problem: A Molecular Dive into PETase Enzyme for Sustainable Recycling
Lindau, Germany — July **2024**

3. **Federation of European Biochemical Society (FEBS): Computational Approaches to Understanding and Engineering Enzyme Catalysis**
Exploring the Light-Emitting Agents in Renilla Luciferases Through Quantum Mechanical Consistent Force Field (QCFF/PI) Method
Zagreb, Croatia — September **2023**

2. **The Physical Organic Chemistry (TPOC) Virtual Meeting**
Isotope-Controlled Selectivity by Quantum Tunneling: Hydrogen Migration versus Ring Expansion in Cyclopropylmethyl Carbenes
UC Davis, USA — August **2021**

1. **85th Annual Meeting of the Israel Chemical Society**
Carbon Tunneling in the Automerization of Cyclo[18]Carbon
Jerusalem, Israel — February **2021**

Academic Contributions

Reviewing Activities

Since 2022 Reviewer for internationally recognized journals:

- *Chemistry - A European Journal*
- *ChemPlusChem*
- *Physical Chemistry Chemical Physics*
- *Helvetica Chimica Acta*
- *European Journal of Organic Chemistry*
- *Inorganic Chemistry*
- *Canadian Journal of Chemistry*
- *Journal of Organic Chemistry*

Other Professional Activities

2022- System administrator and manager of HPC server in the Warshel Research Group.

2022 Participated in the NSF Research Grant ($1.5M) Proposal Writing on "QM/MM *ab initio* free energy surfaces and CG simulations of Biological Processes" with **PI** (Prof. Warshel).

References

Prof. Arieh Warshel
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