

Ashim Nandi

Postdoctoral Research Associate

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Professional Experience

- 2022-** **Research Associate** University of Southern California, USA.
Advisor: Dr. Arie Warshel (Distinguished Professor, and 2013 Chemistry Nobel Laureate).
- 2021-2022** **Postdoctoral Fellow** Weizmann Institute of Science, Israel.
Advisor: Dr. Jan (Gershon) 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** Invitation as a Young Scientist to the 73rd Lindau Nobel Laureate Meetings, 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 Dibenzylidene 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**
Lindau, Germany – July 2024
3. **Federation of European Biochemical Society (FEBS): Computational Approaches to Understanding and Engineering Enzyme Catalysis**
Zagreb, Croatia – September 2023
2. **The Physical Organic Chemistry (TPOC) Virtual Meeting**
UC Davis, USA – August 2021
1. **85th Annual Meeting of the Israel Chemical Society**
Jerusalem, Israel – February 2021

Academic Contributions

Reviewing Activities.....

Since 2022 Reviewer for internationally recognized journals:

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| ○ Chemistry - A European Journal | ○ Physical Chemistry Chemical Physics |
| ○ ChemPlusChem | ○ Helvetica Chimica Acta |

○ *European Journal of Organic Chemistry*

○ *Inorganic Chemistry*
○ *Canadian Journal of 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 on “QM/MM *ab initio* free energy surfaces and CG simulations of Biological Processes” with **PI** (Prof. Warshel).

References

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