

# ODED HOD – curriculum vitae

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## Contact Information

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## Personal Details

- Date of Birth: 23.4.1973
- Place of Birth: Tel-Aviv, Israel.
- Marital status: married to Adi, father of Ophir, Ariel, and Elah.
- Nationality: Israeli.

## Research Interests

- Theoretical and computational study of the physical properties of materials at the nanoscale.
- Electronic properties and transport phenomena of large molecular systems and nanostructures.
- Time-domain simulations of electronic transport through molecular architectures.
- Non-equilibrium electron dynamics and thermodynamics in open quantum systems.
- The role of magnetic and electric fields in nanoscale conductance measurements.
- Dedicated force fields for modeling of complex layered materials interfaces.
- Nanotribology and superlubricity in homogeneous and heterogeneous layered materials interfaces.

## Research Experience

Years	Institution	Area of specialization	Experience
2005-2008	Rice University	Computational Chemistry	Post-Doctoral Research Associate
2008-	Tel-Aviv University	Computational Material Science	Faculty

## Education

Years	Institution	Area of specialization	Degree
2000-2005	Tel-Aviv University	Theoretical Chemistry	Ph.D. (Direct)
1991-1994	Hebrew University	Chemistry and Physics	B.Sc.

## Honors and Awards

Year	Award
2024	Received the Rector's Prize for Teaching Innovation and Creativity.
2022	Israel Chemical Society Tenne Family Prize in Memory of Lea Tenne for Nanoscale Sciences.
2021	The Heineman Chair of Physical Chemistry.
2019	Received the Rector's Award for Excellence in Teaching.
2017	Recipient of the Kadar Family Award for Outstanding Research.
2017	Received the Rector's Award for Excellence in Teaching.
2015	Received the Rector's Award for Excellence in Teaching.
2012	Elected as a Member of the Israeli Young Academy.
2012	Received the Rector's Award for Excellence in Teaching.
2011	Elected as a Member of the Global Young Academy.
2010	Elected as a Member of the Lise Meitner-Minerva Center for Computational Quantum Chemistry.
2005	Fulbright Postdoctoral Fellowship.
2005	Rothschild Postdoctoral Fellowship.
2003	Salim and Rachel Banin Award for outstanding graduate students.

- 2003 Don and Sara Marejn Foundation Award.
- 1995 B.Sc. Magna Cum Laude.
- 1994 Dean's List of Outstanding Scholars.
- 1993 Dean's List of Outstanding Scholars.
- 1992 Dean's List of Outstanding Scholars.
- 1991 Award for outstanding undergraduate candidacy.

## Academic Service

- arXiv Moderator of the Physics.Chem-Ph category.
- Previous Director of Tel-Aviv University's CECAM-ISR Node.
- Reviewed for many peer reviewed journals including: Nano Letters, Physical Review Letters, Journal of the American Chemical Society, Proceedings of the National Academy of Sciences, Physical Review B, The Journal of Physical Chemistry, Journal of Chemical Theory and Computation, Structural Chemistry, and ACS Nano.

## Publications

- 116. Y. Chen, **O. Hod**, J. Gersten, and A. Nitzan, "Chirality-Induced Orbital-Angular-Momentum Selectivity in Electron Transmission and Scattering", submitted (2025).
- 115. X. Gao, W. Ouyang, L. Kronik, M. Urbakh, and **O. Hod**, "Anisotropic Interlayer Force Fields for van der Waals Interfaces: Development and Applications", *J. Chem. Phys.*, in press (2025).
- 114. X. Gao, W. Yan, W. Ouyang, Z. Liu, M. Urbakh, and **O. Hod**, "Frictional Dissipation and Scaling Laws at van der Waals Interfaces: The Role of Edge and Corner Elastic Moiré Pinning", submitted (2025).
- 113. P. Ying, X. Gao, D. Berman, **O. Hod**, and M. Urbakh, "Scaling-up of Structural Superlubricity: Challenges and Opportunities", *Adv. Funct. Mater.*, in press (2025).
- 112. C. Y. Cheng, G. Harari, I. Rončević, J. E. Peralta, H. L. Anderson, A. M. Wibowo-Teale, and **O. Hod**, "Molecular Aharonov-Bohm-Type Interferometers Based on Porphyrin Nanorings", *Chem. Sci.* **16**, 4392-4401 (2025).
- 111. N. Brown, M. Camarasa-Gómez, A. Niazov-Elkan, A. Ramasubramaniam, E. Gazit, L. Kronik, and **O. Hod**, "Role of metal atoms in the refractivity of cysteine- and phenylalanine-based metal-organic crystals", *Mater. Adv.* **6**, 1144-1151 (2025).
- 110. W. Jiang, R. Sofer, X. Gao, L. Kronik, **O. Hod**, M. Urbakh, and W. Ouyang, "Anisotropic Interlayer Force Field for Heterogeneous Interfaces of Graphene and *h*-BN with Transition Metal Dichalcogenides", *J. Phys. Chem. C* **129**, 1417-1427 (2025).
- 109. P. Ying, **O. Hod**, and M. Urbakh, "Superlubric Graphullerene", *Nano Lett.* **24**, 10599-10604 (2024).
- 108. P. Ying, X. Gao, A. Natan, M. Urbakh, and **O. Hod**, "Chemifrication and Superlubricity: Friends or Foes?", *J. Phys. Chem. Lett.* **16**, 2934-2941 (2025).
- 107. A. Silva, X. Gao, M. M. Gianetti, R. Guerra, N. Manini, A. Vanossi, M. Urbakh, and **O. Hod**, "Emerging Chirality and Moiré Dynamics in Twisted Layered Material Heterostructures", *ACS Nano* **18**, 30957-30965 (2024).

106. P. Ying, A. Natan, **O. Hod**, and M. Urbakh, "Effect of Interlayer Bonding on Superlubric Sliding of Graphene Contacts: A Machine-Learning Potential Study", *ACS Nano* **18**, 10133-10141 (2024).
105. W. Cao, S. Deb, M. Vizner Stern, N. Raab, M. Urbakh, **O. Hod**, L. Kronik, and M. Ben Shalom, "Polarization Saturation in Multilayered Interfacial Ferroelectrics", *Adv. Mater.* **36**, 2400750 (2024).
104. Y. Song, X. Gao, R. Pawlak, S. Huang, A. Hinaut, T. Glatzel, **O. Hod**, M. Urbakh, and E. Meyer, "Non-Amontons Frictional Behaviors of Grain Boundaries at Layered Material Interfaces", *Nat. Commun.* **15**, 9487 (2024).
103. **O. Hod** and M. Urbakh, "Uncovering the Secrets of Hidden Twists", *Natl. Sci. Rev.* **10**, nwad215 (2023).
102. W. Jiang, R. Sofer, X. Gao, A. Tkatchenko, L. Kronik, W. Ouyang, M. Urbakh, and **O. Hod**, "Anisotropic Interlayer Force Field for Group-VI Transition Metal Dichalcogenides", *J. Phys. Chem. A* **127**, 9820-9830 (2023).
101. Y. Chen and **O. Hod**, "Chirality Induced Spin Selectivity: A Classical Spin-off", *J. Chem. Phys.* **158**, 244102 (2023).
100. B. Lyu, J. Chen, S. Wang, S. Lou, P. Shen, J. Xie, L. Qiu, I. Mitchell, C. Li, C. Hu, X. Zhou, K. Watanabe, T. Taniguchi, X. Wang, J. Jia, Q. Liang, G. Chen, T. Li, S. Wang, W. Ouyang, **O. Hod**, F. Ding, M. Urbakh, Z. Shi, "Graphene nanoribbons grown in hBN stacks for high-performance electronics", *Nature* **628**, 758-764 (2024).
99. **O. Hod** and L. Kronik, "The Driven Liouville von Neumann Approach to Electron Dynamics in Open Quantum Systems", *Isr. J. Chem.* **63**, e202300058 (2023).
98. W. Cao, M. Urbakh, and **O. Hod**, "Nanotube Slidetronics", *J. Phys. Chem. Lett.* **15**, 9-14 (2024).
97. A. Oz, A. Nitzan, **O. Hod**, and J. E. Peralta, "Electron Dynamics in Open Quantum Systems: The Driven Liouville-von Neuman Methodology within Time Dependent Density Functional Theory", *J. Chem. Theory Comput.* **19**, 7496-7504 (2023).
96. S. Salleh Atri, W. Cao, B. Alon, N. Roy, M. Vizner Stern, V. Falko, M. Goldstein, L. Kronik, M. Urbakh, **O. Hod**, M. Ben Shalom, "Spontaneous Electric Polarization in Graphene Polytypes", *Adv. Phys. Res.* **2300095** (2024).
95. Y. Chen, L. Xu, M. Urbakh, and **O. Hod**, "Spatial Separation of Enantiomers by Field-Modulated Surface Scattering", *J. Phys. Chem. C* **127**, 10997-11004 (2023).
94. W. Yan, X. Gao, W. Ouyang, Z. Liu, **O. Hod**, and M. Urbakh, "Shape-Dependent Friction Scaling Laws in Twisted Layered Material Interfaces", *J. Mech. Phys. Solids* **185**, 105555 (2024).
93. Y. Song, X. Gao, A. Hinaut, S. Scherb, S. Huang, T. Glatzel, **O. Hod**, M. Urbakh, and E. Meyer, "Velocity Dependence of Moiré Friction", *Nano Lett.* **22**, 9529-9536 (2022).
92. W. Cao, **O. Hod**, and M. Urbakh, "Interlayer Registry Dictates Interfacial 2D Material Ferroelectricity", *ACS Appl. Mater. Interfaces* **14**, 57492-57499 (2022).

91. S. Deb, W. Cao, N. Raab, K. Watanabe, T. Taniguchi, M. Goldstein, L. Kronik, M. Urbakh, **O. Hod**, M. Ben Shalom, "Cumulative Polarization in Conductive Interfacial Ferroelectrics", *Nature* **612**, 465-469 (2022).
90. X. Gao, M. Urbakh, and **O. Hod**, "Stick-Slip Dynamics of Moiré Superstructures in Polycrystalline 2D Material Interfaces", *Phys. Rev. Lett.* **129**, 276101 (2022).
89. W. Cao, **O. Hod**, and M. Urbakh, "Interlayer Registry Index of Layered Transition Metal Dichalcogenides", *J. Phys. Chem. Lett.* **13**, 3353-3359 (2022).
88. B. Lyu, J. Chen, S. Lou, C. Li, L. Qiu, W. Ouyang, J. Xie, I. Mitchell, T. Wu, A. Deng, C. Hu, X. Zhou, P. Shen, S. Ma, Z. Wu, K. Watanabe, T. Taniguchi, X. Wang, Q. Liang, J. Jia, M. Urbakh, **O. Hod**, F. Ding, S. Wang, Z. Shi, "Catalytic Growth of Ultralong Graphene Nanoribbons on Insulating Substrates", *Adv. Mater.* **34**, 2200956 (2022).
87. F. Evers, A. Aharony, N. Bar-Gill, O. Entin-Wohlman, P. Hedegård, **O. Hod**, P. Jelinek, G. Kamieniarz, M. Lemeshko, K. Michaeli, V. Mujica, R. Naaman, Y. Paltiel, S. Refaely-Abramson, O. Tal, J. Thijssen, M. Thoss, J. M. van Ruitenbeek, L. Venkataraman, D. H. Waldeck, B. Yan, and L. Kronik, "Theory of Chirality Induced Spin Selectivity: Progress and Challenges", *Adv. Mater.* **34**, 2106629 (2022).
86. **O. Hod** and M. Urbakh, "Sliding on the Edge", *Nat. Mater. (News & Views)* **21**, 12-14 (2022).
85. W. Ouyang, R. Sofer, X. Gao, J. Hermann, A. Tkatchenko, L. Kronik, M. Urbakh, and **O. Hod**, "Anisotropic Interlayer Force Field for Transition Metal Dichalcogenides: The Case of Molybdenum Disulfide", *J. Chem. Theory Comput.* **17**, 7237-7245 (2021).
84. W. Ouyang, **O. Hod**, and R. Guerra, "Registry Dependent Potential for Interfaces of Gold with Graphitic Systems", *J. Chem. Theory Comput.* **17**, 7215-7223 (2021).
83. W. Ouyang, **O. Hod**, and M. Urbakh, "Registry Dependent Peeling of Layered Material Interfaces: The Case of Graphene Nanoribbons on Hexagonal Boron Nitride", *ACS Appl. Mater. Interfaces* **13**, 43533-45359 (2021).
82. A. Oz, D. Dutta, A. Nitzan, **O. Hod**, and E. Koren, "Edge State Quantum Interference in Twisted Graphitic Interfaces", *Adv. Sci.* **9**, 2102261 (2022).
81. X. Gao, W. Ouyang, M. Urbakh, and **O. Hod**, "Superlubric Polycrystalline Graphene Interfaces", *Nat. Commun.* **12**, 5694 (2021).
80. W. Ouyang, **O. Hod**, and M. Urbakh, "Parity-Dependent Moiré Superlattices in Graphene/h-BN Heterostructures: A Route to Mechanomutable Metamaterials", *Phys. Rev. Lett.* **126**, 216101 (2021).
79. M. Vizner Stern, Y. Waschitz, W. Cao, I. Nevo, K. Watanabe, T. Taniguchi, E. Sela, M. Urbakh, **O. Hod**, and M. Ben Shalom, "Interfacial Ferroelectricity by van der Waals Sliding", *Science* **372**, 1462-1466 (2021).
78. W. Ouyang, H. Qin, M. Urbakh, and **O. Hod**, "Controllable Thermal Conductivity in Twisted Homogeneous Interfaces of Graphene and Hexagonal Boron Nitride", *Nano Lett.* **20**, 7513-7518 (2020).
77. S. Rozen, I. Vints, A. Lerner, **O. Hod**, E. N. Brothers, and S. Moncho, "The Chemistry of Short-Lived  $\alpha$ -Fluorocarboxocations", *J. Org. Chem.* **86**, 3882-3889 (2021).

76. S. Chakrabarti, A. Vilan, G. Deutch, A. Oz, **O. Hod**, J. E. Peralta, and O. Tal, "Magnetic Control Over the Fundamental Structure of Atomic Wires", *Nat. Commun.* **13**, 4113 (2022).
75. A. K. Mondal, N. Brown, S. Mishra, P. Makam, D. Wing, S. Gilead, Y. Wiesenfeld, G. Leituss, L. J. W. Shimon, R. Carmieli, D. Ehre, G. Kamieniarz, J. Fransson, **O. Hod**, L. Kronik, E. Gazit, and R. Naaman, "Long-Range Spin-Selective Transport in Chiral Metal-Organic Crystals with Temperature-Activated Magnetization", *ACS Nano* **14**, 16624-16633 (2020).
74. X. Gao, W. Ouyang, **O. Hod**, and M. Urbakh, "Mechanisms of Frictional Energy Dissipation at Graphene Grain Boundaries", *Phys. Rev. B* **103**, 045418 (2021).
73. D. Dutta, A. Oz, **O. Hod**, and E. Koren, "The Scaling Laws of Edge vs. Bulk Interlayer Conduction in Mesoscale Twisted Graphitic Interfaces", *Nat. Commun.* **11**, 4746 (2020).
72. A. Oz, **O. Hod**, and A. Nitzan, "Numerical Approach to Non-Equilibrium Quantum Thermodynamics: Nonperturbative Treatment of the Driven Resonant Level Model Based on the Driven Liouville von-Neumann Formalism", *J. Chem. Theory Comput.* **16**, 1232-1248 (2020).
71. W. Ouyang, I. Azuri, D. Mandelli, A. Tkatchenko, L. Kronik, M. Urbakh, and **O. Hod**, "Mechanical and Tribological Properties of Layered Materials Under High Pressure: Assessing the Importance of Many-Body Dispersion Effects", *J. Chem. Theory Comput.* **16**, 666-676 (2020).
70. T. Maaravi and **O. Hod**, "Simulating Electron Dynamics in Open Quantum Systems under Magnetic Fields", *J. Phys. Chem. C* **124**, 8652-8662 (2020).
69. D. Mandelli, W. Ouyang, M. Urbakh, and **O. Hod**, "The Princess and the Nanoscale Pea: Long-Range Penetration of Surface Distortions into Layered Materials Stacks", *ACS Nano* **13**, 7603-7609 (2019).
68. I. Oz, **O. Hod**, and A. Nitzan, "Evaluation of Dynamical Properties of Open Quantum Systems Using the Driven Liouville-von Neumann Approach: Methodological Considerations", *Mol. Phys.* **117**, 2083-2096 (2019).
67. D. Mandelli, W. Ouyang, **O. Hod**, M. Urbakh, "Negative Friction Coefficient in Superlubric Graphite-Hexagonal Boron Nitride Heterojunctions", *Phys. Rev. Lett.* **122**, 076102 (2019).
66. W. Ouyang, D. Mandelli, M. Urbakh, **O. Hod**, "Nanoserpents: Graphene Nanoribbon Motion on Two-Dimensional Hexagonal Materials", *Nano Lett.* **18**, 6009-6016 (2018).
65. **O. Hod**, M. Urbakh, D. Naveh, M. Bar-Sadan, and A. Ismach, "Flatlands in the Holy Land: The Evolution of Layered Materials Research in Israel", *Adv. Mater.* **30**, 1706581 (2018).
64. I. Azuri, A. Hirsch, A. M. Reilly, A. Tkatchenko, S. Kendler, **O. Hod**, and L. Kronik, "TeraHertz Spectroscopy of 2,4,6-trinitrotoluene Molecular Solids from First Principles", *Beilstein J. Org. Chem.* **14**, 381-388 (2018).
63. Y. Song, D. Mandelli, **O. Hod**, M. Urbakh, M. Ma, and Q. Zheng, "Robust Microscale Superlubricity in Graphite/Hexagonal Boron Nitride Layered Heterojunctions", *Nat. Mater.* **17**, 894-899 (2018).
62. T. Maaravi, I. Leven, I. Azuri, L. Kronik, and **O. Hod**, "Interlayer Potential for Homogeneous Graphene and Hexagonal Boron Nitride Systems: Reparameterization for Many-Body Dispersion Effects", *J. Phys. Chem. C* **121**, 22826-22835 (2017).

61. L. Adler-Abramovich, Z. Arnon, X.-M. Sui, I. Azuri, H. Cohen, **O. Hod**, L. Kronik, L. J. W. Shimon, H. D. Wagner, and E. Gazit, "Bioinspired Flexible and Tough Layered Peptide Crystals", *Adv. Mater.* **30**, 1704551 (2018).
60. **O. Hod**, E. Meyer, Q. Zheng, and M. Urbakh, "Structural Superlubricity and Ultralow Friction Across the Length Scales", *Nature* **563**, 485-492 (2018).
59. R. Guerra, I. Leven, A. Vanossi, **O. Hod**, and E. Tosatti, "Smallest Archimedean Screw: Facet Dynamics and Friction in Multi-Walled Nanotubes", *Nano Lett.* **17**, 5321-5328 (2017).
58. D. Mandelli, I. Leven, **O. Hod**, and M. Urbakh, "Sliding Friction of Graphene/Hexagonal-Boron Nitride Heterojunctions: A Route to Robust Superlubricity", *Sci. Rep.* **7**, 10851 (2017).
57. T. Zelovich, T. Hansen, Z.-F. Liu, J. B. Neaton, L. Kronik, and **O. Hod**, "Parameter Free Driven Liouville–von Neumann Approach for Time-Dependent Electronic Transport Simulations in Open Quantum Systems", *J. Chem. Phys.* **146**, 092331 (2017).
56. D. Krepel and **O. Hod**, "Selectivity of a Graphene Nanoribbon-Based Trinitrotoluene Detector: A Computational Assessment", *J. Phys. Chem. C* **121**, 21546-21552 (2017).
55. T. Zelovich, L. Kronik, and **O. Hod**, "Driven Liouville von Neumann Approach for Time-Dependent Electronic Transport Calculations in a Nonorthogonal Basis-Set Representation", *J. Phys. Chem. C* **120**, 15052–15062 (2016).
54. I. Leven, T. Maaravi, I. Azuri, L. Kronik, and **O. Hod**, "Inter-Layer Potential for Graphene/*h*-BN Heterostructures", *J. Chem. Theory Comput.* **12**, 2896-2905 (2016).
53. I. Leven, R. Guerra, A. Vanossi, E. Tosatti, and **O. Hod**, "Multiwalled Nanotube Faceting Unravelling", *Nat. Nanotechnol.* **11**, 1082-1086 (2016).
52. I. Oz, I. Leven, Y. Itkin, A. Buchwalter, K. Akulov, and **O. Hod**, "Nanotube Motion on Layered Materials: A Registry Perspective", *J. Phys. Chem. C* **120**, 4466-4470 (2016). arXiv:1512.08612.
51. **O. Hod**, C. A. Rodríguez-Rosario, T. Zelovich, and T. Frauenheim, "Driven Liouville von Neumann Equation in Lindblad Form", *J. Phys. Chem. A* **120**, 3278-3285 (2016). arXiv:1512.05862.
50. D. Krepel, J. E. Peralta, G. E. Scuseria, and **O. Hod**, "Graphene Nanoribbons-Based Ultrasensitive Chemical Detectors", *J. Phys. Chem. C* **120**, 3791-3797 (2016).
49. E. Koren, I. Leven, E. Lörtscher, A. Knoll, **O. Hod**, and U. Duerig, "Coherent Commensurate Electronic States at the Interface Between Misoriented Graphene Layers", *Nat. Nanotechnol.* **11**, 752-757 (2016).
48. R. Pawlak, W. Ouyang, A. E. Filippov, L. Kalikhman-Razvozov, S. Kawai, T. Glatzel, E. Gneco, A. Baratoff, Q. Zheng, **O. Hod**, M. Urbakh, and E. Meyer, "Single Molecule Tribology: Force Microscopy Manipulation of a Porphyrin Derivative on a Copper Surface", *ACS Nano* **10**, 713-722 (2016).
47. T. Zelovich, L. Kronik, and **O. Hod**, "Molecule-Lead Coupling at Molecular Junctions: Relation Between the Real- and State-Space Perspectives", *J. Chem. Theory Comput.*, **11**, 4861-4869 (2015).

46. J. E. Peralta, **O. Hod**, and G. E. Scuseria, "Magnetization Dynamics From Time-Dependent Non-Collinear Spin Density Functional Theory Calculations", *J. Chem. Theory Comput.* **11**, 3661–3668 (2015).
45. D. Krepel, L. Kalikhman-Razvozov, and **O. Hod**, "Edge Chemistry Effects on the Structural, Electronic, and Electric Response Properties of Boron Nitride Quantum Dots", *J. Phys. Chem. C* **118**, 21110-21118 (2014). arXiv:1404.4264.
44. T. Zelovich, L. Kronik, and **O. Hod**, "State Representation Approach for Atomistic Time-Dependent Transport Calculations in Molecular Junctions", *J. Chem. Theory Comput.* **10**, 2927-2941 (2014). arXiv:1402.4906.
43. B. Feldman, T. Seideman, **O. Hod**, and L. Kronik, "Real-Space Method for Highly Parallelizable Electronic Transport Calculations", *Phys. Rev. B* **90**, 035445 (2014). arXiv:1401.0782.
42. I. Leven, I. Azuri, L. Kronik, and **O. Hod**, "Inter-Layer Potential for Hexagonal Boron Nitride", *J. Chem. Phys.* **140**, 104106 (2014). arXiv:1310.2718.
41. N. Brown and **O. Hod**, "Controlling the Electronic Properties of Nanodiamonds via Surface Chemical Functionalization: A DFT Study", *J. Phys. Chem. C* **118**, 5530-5537 (2014). arXiv:1309.3906.
40. D. Krepel and **O. Hod**, "Effects of Edge Oxidation on the Structural, Electronic, and Magnetic Properties of Zigzag Boron Nitride Nanoribbons", *J. Chem. Theory Comput.* **10**, 373-380 (2014). arXiv:1308.1894.
39. D. Krepel and **O. Hod**, "Lithium Mediated Benzene Adsorption on Graphene and Graphene Nanoribbons", *J. Phys. Chem. C* **117**, 19477-19488 (2013). arXiv:1306.2300.
38. I. Azuri, L. Adler-Abramovich, E. Gazit, **O. Hod**, and L. Kronik, "Why are Diphenylalanine-Based Peptide Nanostructures so Rigid? Insights from First Principles Calculations", *J. Am. Chem. Soc.* **136**, 963-969 (2014).
37. A. Hever, J. Bernstein, and **O. Hod**, "Fluorination Effects on the Structural Stability and Electronic Properties of  $sp^3$  Type Silicon Nanotubes", *J. Phys. Chem. C* **117**, 14684-14691 (2013). arXiv:1305.1807.
36. **O. Hod**, "The Registry Index: A Quantitative Measure of Materials Interfacial Commensurability", *ChemPhysChem* **14**, 2376-2391 (2013).
35. L. Kalikhman-Razvozov, R. Yusupov, and **O. Hod**, "Effects of Partial Hydrogenation on the Structure and Electronic Properties of Boron Nitride Nanotubes", *J. Phys. Chem. C* **117**, 22224-22231 (2013). arXiv: 1212.6231.
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33. J. Garel, I. Leven, C. Zhi, K.S. Nagapriya, R. Popovitz-Biro, D. Golberg, Y. Bando, **O. Hod**, and Ernesto Joselevich, "Ultrahigh Torsional Stiffness and Strength of Boron Nitride Nanotubes", *Nano Lett.* **12**, 6347-6352 (2012).
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31. A. Blumberg, U. Keshet, I. Zaltsman, and **O. Hod**, "Interlayer Registry to Determine the Sliding Potential of Layered Metal Dichalcogenides: The Case of  $2H\text{-MoS}_2$ ", *J. Phys. Chem. Lett.* **3**, 1936-1940 (2012). arXiv:1205.3794.
30. **O. Hod**, "Interlayer Commensurability and Superlubricity in Rigid Layered Materials", *Phys. Rev. B* **86**, 075444 (2012). arXiv:1204.3749.
29. D. Rai, **O. Hod**, and A. Nitzan, "Magnetic Fields Effects on the Electronic Conduction Properties of Molecular Ring Structures ", *Phys. Rev. B* **85**, 155440 (2012). arXiv:1109.0619.
28. **O. Hod**, "Graphite and Hexagonal Boron-Nitride Have the Same Interlayer Distance. Why?", *J. Chem. Theory Comput.* **8**, 1360-1369 (2012). arXiv:1109.3813.
27. T. Aqua, H. Cohen, O. Sinai, V. Frydman, T. Bendikov, D. Krepel, **O. Hod**, L. Kronik, and R. Naaman, "Role of Backbone Charge Rearrangement in the Bond-Dipole and Work Function of Molecular Monolayers", *J. Phys. Chem. C* **115**, 24888-24892 (2011).
26. N. Marom, A. Tkatchenko, M. Rossi, V. V. Gobre, **O. Hod**, M. Scheffler, and L. Kronik, "Dispersion Interactions with Density-Functional Theory: Benchmarking Semi-Empirical and Inter-Atomic Pair-Wise Corrected Density Functionals", *J. Chem. Theory Comput.* **7**, 3944-3951 (2011).
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23. Dana Krepel and **O. Hod**, "Lithium Adsorption on Armchair Graphene Nanoribbons", *Surf. Sci.* **605**, 1633-1642 (2011). (Invited article: special issue on "Graphene").
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15. N. Marom, **O. Hod**, G. E. Scuseria, and L. Kronik, "Electronic Structure of Copper Phthalocyanine: a Comparative Density Functional Theory Study", *J. Chem. Phys.* **128**, 164107 (2008). arXiv:0801.0733.
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  12. **O. Hod**, V. Barone, J. E. Peralta, and G. E. Scuseria, "Enhanced Half-Metallicity in Edge-Oxidized Zigzag Graphene Nanoribbons", *Nano Lett. (Letter)* **7**, 2295-2299 (2007). arXiv:0704.2043.
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  2. **O. Hod** and E. Rabani, "A Coarse-Grained Model for a Nanometer Scale Molecular Pump", *Proc. Natl. Acad. Sci. USA* **100**, 14661-14665 (2003).
  1. **O. Hod**, E. Rabani, and R. Baer, "Carbon Nanotube Closed Ring Structures", *Phys. Rev. B* **67**, 195408 (2003).
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5. **O. Hod**, "Slippery science" in "The Israel Chemist and Chemical Engineer - Issue 10" (Editor Arlene D. Wilson-Gordon), DOI: <https://doi.org/10.51167/ice00000> (Israel Chemical Society, 2024).

4. **O. Hod**, M. Urbakh, and D. Berman (2024). "The (Grain) Boundaries of Structural Superlubricity". In: E. Gnecco and E. Meyer (Eds.) **"Fundamentals of Friction and Wear on the Nanoscale"**. NanoScience and Technology. Springer, Cham. [https://doi.org/10.1007/978-3-031-63065-1\\_5](https://doi.org/10.1007/978-3-031-63065-1_5)
3. **O. Hod**, "Interlayer Interactions in Low-Dimensional Layered Hetero-Structures: Modeling and Applications" in **"Handbook of Materials Modeling. Volume 2 Applications: Current and Emerging Materials"** (Editors-in-chief Wanda Andreoni and Sidney Yip), Section 4: **"Emergent Systems with Limited Dimensionality"** (section Editor James R. Chelikowsky), DOI: [https://doi.org/10.1007/978-3-319-50257-1\\_38-1](https://doi.org/10.1007/978-3-319-50257-1_38-1) (Springer, 2018).
2. D. Krepel and **O. Hod**, "Physical Properties of Graphene Nanoribbons: Insights from First-Principles Studies" chapter 4 in **"Graphene Chemistry: Theoretical Perspectives"** (Ed. De-en Jiang and Zhongfang Chen) 51-77 (John Wiley & Sons, Inc., Chichester, UK, 2013).
1. V. Barone, **O. Hod**, and J. E. Peralta, "Modeling of Quasi-One-Dimensional Carbon Nanostructures with Density Functional Theory" in **"Handbook of Computational Chemistry"** (Ed. Jerzy Leszczynski), Vol 2: **"Solid States and Nanomaterials"** (Eds. Manthos G. Papadopoulos and Heribert Reis) 901-938 (Springer, 2012).

## Teaching Experience

Lecturer of the following undergraduate and graduate courses of the school of chemistry at the Tel-Aviv University:

2022-	Quantum Dynamics
2019-24	Thermodynamics
2016-19	Statistical Thermodynamics
2010-16	Introduction to Quantum Mechanics and the Chemical Bond
2009-17, 19, 24	Quantum Chemistry

Teaching Assistant of the following undergraduate courses of the school of chemistry at the Tel-Aviv University:

2003-2005	Physical Chemistry II – Quantum Mechanics and spectroscopy.
2002-2004	Physical Chemistry I – Thermodynamics and kinetics.

Received outstanding reviews in official teaching evaluation surveys.

## Symposia & Presentations

"Structural Superlubricity: from Growth Selectivity to Defect Healing" – Invited talk - 5<sup>th</sup> Meeting of the Israeli Conference on Computational Modelling of Molecules and Solids (CMMS), Ramat Gan, Israel (July 15<sup>th</sup> 2025).

"Layered Ferroelectricity: from Geometric Measures to First-Principles Calculations" – Invited talk – "2D Materials" session, The 20<sup>th</sup> Israel Materials Engineering Conference (IMEC20), Jerusalem, Israel (February 25<sup>th</sup> 2025).

"Structural Superlubricity: from Growth Selectivity to Defect Healing" – Plenary talk - 2025 Structural Superlubricity Conference (SSL 2025), Shenzhen, China (January 20<sup>th</sup> 2025).

"The Fascinating Frictional Properties of Layered Materials" – Invited talk – Department of Chemical Engineering - departmental Seminar, Be'er Seva, Israel (November 19<sup>th</sup> 2024).

"Structural Superlubricity: from Growth Selectivity to Defect Healing" – Invited talk – 1<sup>st</sup> Israeli Conference on Tribology and Biotribology, Jerusalem, Israel (October 29<sup>th</sup> 2024).

"Layered Ferroelectricity: from Geometric Measures to First-Principles Calculations" – Keynote lecture – "Nanoscience for Future Quantum Technologies: Novel Materials, Devices, and Characterizations" session, IVS-IPSTA - 41<sup>st</sup> Annual Conference, Tel Aviv, Israel (October 28<sup>th</sup> 2024).

"Layered Ferroelectricity: from Geometric Measures to First-Principles Calculations" – Invited talk – 87<sup>th</sup> Israel Chemical Society Meeting, Tel Aviv, Israel (April 3<sup>rd</sup> 2024).

"Chirality Induced Spin Selectivity: A Classical Spin-Off" – Invited Webinar – Fransson CISS biweekly webinar series, Uppsala University, Sweden (January 17<sup>th</sup> 2024).

"Layered Ferroelectricity: from Geometric Measures to First-Principles Calculations" – Invited Webinar - Nanotribology Webinar, School of Mechanical Engineering, Southeast University, Nanjing, China (November 27<sup>th</sup> 2023).

"Layered Ferroelectricity: from Geometric Measures to First-Principles Calculations" – Invited (online) talk - Condensed Matter Physics & Nanotribology – Conference in Honor of Erio Tosatti, Trieste, Italy (November 15<sup>th</sup> 2023).

Session chair, "2DM - 2D Materials & Layered Materials", 36<sup>th</sup> European Conference on Surface Science (ECOSS36), Lodz, Poland (August 31<sup>st</sup> 2023).

"Layered Ferroelectricity: from Geometric Measures to First-Principles Calculations" – Invited talk - 36<sup>th</sup> European Conference on Surface Science (ECOSS36), Lodz, Poland (August 30<sup>th</sup> 2023).

Session chair, Electronic Transport in Molecular Quantum Conductors, Rehovot, Israel (June 29<sup>th</sup> 2023).

"The Driven Liouville von Neumann (DLvN) Approach for Electron Dynamics in Open Quantum Systems" – Invited Talk – Electronic Transport in Molecular Quantum Conductors, Rehovot, Israel (June 28<sup>th</sup> 2023).

"The Driven Liouville von Neumann (DLvN) Approach for Electron Dynamics in Open Quantum Systems" – Invited Talk – CECAM Flagship School on Path Integral Quantum Mechanics, Tel Aviv, Israel (June 7<sup>th</sup> 2023).

Session chair, CECAM Flagship School on Path Integral Quantum Mechanics, Tel Aviv, Israel (June 5<sup>th</sup> 2023).

"Layered Ferroelectricity - from Geometric Measures to First-Principles Calculations" – Invited Talk – Twistronics 2023 – International Workshop on twisted bilayer graphene and beyond, Seoul, S. Korea (January 12<sup>th</sup> 2023).

"The Fascinating Frictional Properties of Layered Materials" – Online Invited Talk – Friction, lubrication and rheology at the nano and mesoscale, Durham, England (July 20<sup>th</sup> 2022).

"Structural Superlubricity Meets Grain Boundaries" – Invited Talk – 7<sup>th</sup> World Tribology Congress 2022 – Fundamentals of Friction theme, Lyon, France (July 13<sup>th</sup> 2022).

"The Fascinating Frictional Properties of Layered Materials" – Invited Talk – the 4<sup>th</sup> Tel Aviv University - Northwestern University Workshop, Tel Aviv, Israel (June 22<sup>nd</sup> 2022).

Session co-chair, "Simulating Moiré Interfaces", Quantum Materials Design by vdW Stacking, Sliding, and Twisting, Tel Aviv, Israel (June 13<sup>th</sup> 2022).

"MD Simulations of Layered Materials" – Invited Talk (Tutorial) – Quantum Materials Design by vdW Stacking, Sliding, and Twisting, Tel Aviv, Israel (June 13<sup>th</sup> 2022).

"The Fascinating Frictional Properties of Layered Materials" – Invited Talk – IPS Conference 2022 - the 67<sup>th</sup> Annual Meeting of the Israel Physical Society, Beersheba, Israel (February 22<sup>nd</sup> 2022).

"The Fascinating Frictional Properties of Layered Materials" – Invited Talk – IMEC2021 - the 19<sup>th</sup> Israel Materials Engineering Conference, Jerusalem, Israel (December 13<sup>th</sup> 2021).

Session co-chair, "2D Materials", Nano.IL.2021 - the international nanotechnology conference in Israel, Jerusalem, Israel (October 5<sup>th</sup> 2021).

"The Fascinating Frictional Properties of Layered Materials" – Invited Talk – Nano.IL.2021 - the international nanotechnology conference in Israel, Jerusalem, Israel (October 5<sup>th</sup> 2021).

"The Fascinating Frictional Properties of Layered Materials" – Online Invited Talk – Hebrew University of Jerusalem – Fritz-Haber Center for Molecular Dynamics Seminar (May 6<sup>th</sup> 2021).

"Controllable Properties of Graphene and Hexagonal Boron Nitride Stacks: A Route to Programmable Metamaterials" – Online Pitch Talk – Tel Aviv University - University of Potsdam Biological and Soft Matter Online Meeting on "Programmable Nanomaterials and Interfaces" (November 23<sup>rd</sup> 2020).

"Modeling Interlayer Interactions in Layered Materials" – Online Invited Talk – Departmental Seminar, Sde Boker, Israel (June 9<sup>th</sup> 2020).

"Modeling Interlayer Interactions in Layered Materials" – Keynote Lecture – CECAM Workshop on "Molecular Mechanisms of Tribochemistry and Lubrication", Lausanne, Switzerland (January 29<sup>th</sup> 2020).

"Chiral Induced Spin Selectivity: A Classical Analogue" – Invited Talk – Workshop on "The Theory of CISS", Rehovot, Israel (January 13<sup>th</sup> 2020).

"Modeling Interlayer Interactions in Layered Materials" – Invited Talk – Israel-Italy Workshop on 2D Materials, Ramat Gan, Israel (November 27<sup>th</sup> 2019).

Co-organizer of the Israel-Italy Workshop on 2D Materials, Ramat Gan, Israel (November 25<sup>th</sup> – November 27<sup>th</sup> 2019).

"The Fascinating Frictional Properties of Layered Materials: Insights from Atomistic Modeling - I", 2<sup>nd</sup> International Workshop on Superlubricity at Nano and Mesoscales, Shenzhen, China (October 16<sup>th</sup> 2019).

"Basic Concepts in Quantum Chemistry" – Invited Talk – CECAM workshop on "From Quantum Computing to Quantum Chemistry: Theory, Platforms, and Practical Applications", Tel Aviv, Israel (September 15<sup>th</sup> 2019).

Co-organizer of the CECAM workshop on "From Quantum Computing to Quantum Chemistry: Theory, Platforms, and Practical Applications", Tel Aviv, Israel (September 15<sup>th</sup> – September 18<sup>th</sup> 2019).

Co-organizer of the Penn Conference in Theoretical Chemistry (PCTC) on "Chemical Dynamics in the Condensed Phase: A Workshop to Honor Abe Nitzan's 75<sup>th</sup> Birthday", Philadelphia, USA (August 12<sup>th</sup> – August 14<sup>th</sup> 2019).

"Modeling Interlayer Interactions in Layered Materials" – Invited Talk – Physical Chemistry Seminar, University of Toronto, Canada (August 7<sup>th</sup> 2019).

"(Non-)Dissipative Dynamics in Nano- and Micro-scale Layered Materials Interfaces" – Invited Talk – CECAM workshop on "Interface Dynamics and Dissipation Across the Time and Length-Scales", Tel Aviv, Israel (May 21<sup>st</sup> 2019).

Session Chair, Nanomaterials session of the Computational Chemistry Symposium, ICCMSE 2019 – 15<sup>th</sup> International Conference of Computational Methods in Sciences and Engineering, Rhodes, Greece (May 3<sup>rd</sup> 2019).

"Modeling Interlayer Interactions in Layered Materials" – Invited Talk – ICCMSE 2019 – 15<sup>th</sup> International Conference of Computational Methods in Sciences and Engineering, Rhodes, Greece (May 3<sup>rd</sup> 2019).

"Modeling Interlayer Interactions in Layered Materials" – Physics Colloquium – Tel Aviv University, Tel Aviv, Israel (April 14<sup>th</sup> 2019).

"Modeling Interlayer Interactions in Layered Materials" – Invited Talk – The Bayreuth-Tel Aviv Workshop on Materials, Tel Aviv, Israel (March 14<sup>th</sup> 2019).

"Modeling Interlayer Interactions in Layered Materials" – Invited Talk – Winter School on 2D Materials, Rehovot, Israel (January 17<sup>th</sup> 2019).

Session Chair, Winter School on 2D Materials, Rehovot, Israel (January 15<sup>th</sup> 2019).

"Electron Dynamics in Open Quantum Systems via The Driven Liouville von Neumann (DLvN) Approach" - Invited Talk – "Quantum Mechanics in Chemistry: From Structure to Dynamics", Haifa, Israel (January 10<sup>th</sup> 2019).

"Modeling Interlayer Interactions in Layered Materials" – Invited Talk – CECAM-Sackler School and Workshop on "Frontiers in Molecular Dynamics: Machine Learning, Deep Learning, and Coarse Graining", Tel Aviv, Israel (October 11<sup>th</sup> 2018).

"Modeling Interlayer Interactions in Layered Materials" – Invited Talk – The 13<sup>th</sup> International Symposium on "Computational Challenges and Tools for Nanotubes" – a parallel session of the 19<sup>th</sup> International Conference on "The Science and Application of Nanotubes and Low-Dimensional Materials", Beijing, China (July 15<sup>th</sup> 2018).

"Modeling Interlayer Interactions in Layered Materials" – Invited Talk – The British Council's UK-Israel Synergy Programme Workshop on "Induced Strain in Atomically Thin Materials", Exeter, UK (July 3<sup>rd</sup> 2018).

Session Chair, "Mechanics Of Multifunctional 2D Materials – Graphene And Beyond", USNC/TAM 2018 – 18<sup>th</sup> US National Congress for Theoretical and Applied Mechanics, Chicago, USA (June 7<sup>th</sup> 2018).

"Modeling Interlayer Interactions in Layered Materials" – Invited Talk – session on "Mechanics Of Multifunctional 2D Materials – Graphene And Beyond", USNC/TAM 2018 – 18<sup>th</sup> US National Congress for Theoretical and Applied Mechanics, Chicago, USA (June 7<sup>th</sup> 2018).

"Electron Dynamics in Open Quantum Systems via The Driven Liouville von Neumann (DLvN) Approach" - Invited Talk - CECAM workshop on "Strongly Correlated Materials: Experiments and Computation", Tel Aviv, Israel (April 11<sup>th</sup> 2018).

Session Chair, "Computational Chemistry Symposium, Materials II Session", ICCMSE 2018 – 14<sup>th</sup> International Conference of Computational Methods in Sciences and Engineering, Thessaloniki, Greece (March 16<sup>th</sup> 2018).

"Modeling Interlayer Interactions in Layered Materials" – Invited Talk – ICCMSE 2018 – 14<sup>th</sup> International Conference of Computational Methods in Sciences and Engineering, Thessaloniki, Greece (March 16<sup>th</sup> 2018).

"Non-Equilibrium Thermodynamics in Open Quantum Systems via The Driven Liouville von Neumann (DLvN) Approach" - Invited Talk - Jerusalem Nonadiabatica 2018: Theory of Nonadiabatic Processes, Jerusalem, Israel (March 12<sup>th</sup> 2018).

Session Chair, "Physical Chemistry I", The 83<sup>rd</sup> Annual Meeting of the Israel Chemical Society, Tel Aviv, Israel (February 13<sup>th</sup> 2018).

"The Driven Liouville von Neumann (DLvN) Approach – Towards a TDDFT Implementation" - Invited Talk - CECAM workshop on "Expeditious Methods in Electronic Structure Theory and Many-Body Techniques", Tel Aviv, Israel (December 19<sup>th</sup> 2017).

"Modeling Interlayer Interactions in Layered Materials" – 6<sup>th</sup> World Tribology Congress 2017 (WTC2017), Beijing, China (September 19<sup>th</sup> 2017).

"Modeling Interlayer Interactions in Layered Materials" – Invited Talk – Joint ICTP-COST-MODPHYSFRICT Conference on "Trends in Nanotribology 2017" (TiN17), Trieste, Italy (June 28<sup>th</sup> 2017).

Co-organizer of the CECAM Tutorial and Workshop on "Bridging the Worlds of Electromagnetic and Quantum Simulations", Tel Aviv, Israel (June 19<sup>th</sup> – June 23<sup>rd</sup> 2017).

"Time Dependent Description of Open Systems and Elements of Quantum Transport" – CECAM Tutorial on "Bridging the Worlds of Electromagnetic and Quantum Simulations", Tel Aviv, Israel (June 19<sup>th</sup> 2017).

"Modeling Interlayer Interactions in Layered Materials" – Invited Talk – Departmental seminar of the Chemistry department at Ben-Gurion University, Beer Sheba, Israel (June 5<sup>th</sup> 2017).

"Global Trends in Funding of Fundamental Research: The Case of Israeli and Canadian Academia" – Invited Talk – "From the Laboratory to the Market and Back?", Historical and Critical Explorations of the Interchange between Academia and Industry, Beer Sheba, Israel (May 8<sup>th</sup> 2017).

"Modeling Interlayer Interactions in Layered Materials" – Invited Talk – Colloquium of the Hebrew University Center for Nanoscience and Nanotechnology, Jerusalem, Israel (March 14<sup>th</sup> 2017).

"Modeling Interlayer Interactions in Layered Materials" – Invited Talk – ISF-NSFC Joint Workshop on Nanoscience and Nanophotonics, Rehovot, Israel (December 5<sup>th</sup> 2016).

"Modeling Interlayer Interactions in Layered Materials" – Invited Talk – 2<sup>nd</sup> Israel-Greece joint meeting on Nanotechnology and Bionanoscience, Crete, Greece (October 27<sup>th</sup> 2016).

"Interlayer Commensurability and Sliding in Layered Materials: the Power of the Registry Index" – Invited Talk – Yeda Fund Seminar on "Nanotechnology and its Applications – Is the Future Already Here?", Eilat, Israel (September 27<sup>th</sup> 2016).

"Research Group Presentation" – Invited Talk - Tsinghua-TAU workshop, Beijing, China (September 20<sup>th</sup> 2016).

"Modeling Interlayer Interactions in Layered Materials" – Invited Talk – 2D Materials School of the Israel Vacuum Society, Rehovot, Israel (September 13<sup>th</sup> 2016).

Co-organizer (together with Prof. Michael Urbakh) of the 2016 Raymond and Beverly Sackler Center for Computational Molecular and Materials Science Summer School and Workshop on "Classical and Quantum Non-Equilibrium Dynamics", Tel Aviv, Israel (August 3<sup>rd</sup>-10<sup>th</sup> 2016).

"Interlayer Commensurability and Sliding in Layered Materials: the Power of the Registry Index" – Invited Talk – 2<sup>nd</sup> Annual NYU-TAU Symposium on "Frontiers in Organized and Nanoscale Matter", New York, USA (June 15<sup>th</sup> 2016).

Session Chair, "Spectroscopy and Dynamics of Materials", The 81<sup>st</sup> Annual Meeting of the Israel Chemical Society, Tel Aviv, Israel (February 9<sup>th</sup> 2016).

"Interlayer Commensurability and Sliding in Layered Materials: the Power of the Registry Index" – Invited Talk – Department of Materials Science and Engineering, Technion – Israel Institute of Technology, Haifa, Israel (January 21<sup>st</sup> 2016).

"A CAP-Based Real-Space Approach for Steady-State Transport Calculations" – Invited Talk – CECAM workshop on "DFT and TDDFT in the Real-Space Formalism within the PARSEC Code: Perspectives and Future Development", Tel Aviv, Israel (December 13<sup>th</sup> – December 17<sup>th</sup> 2015).

Co-organizer of the CECAM workshop on "Open Quantum Systems: Computational Methods", Hong Kong (November 30<sup>th</sup> – December 4<sup>th</sup> 2015).

"Interlayer Commensurability and Sliding in Layered Materials: the Power of the Registry Index" – Invited Talk – "XIN International Workshop on Superlubricity: Fundamentals and Applications", Beijing, China (October 20<sup>th</sup> 2015).

"Interlayer Commensurability and Sliding in Layered Materials: the Power of the Registry Index" – Invited Talk - The 33<sup>rd</sup> Israel Vacuum Society conference - IVS 2015, Rehovot, Israel (September 9<sup>th</sup> 2015).

"Interlayer Commensurability and Sliding in Layered Materials: the Power of the Registry Index" – "Flatlands Beyond Graphene 2015", Ramat Gan, Israel (July 8<sup>th</sup> 2015).

"Interlayer Commensurability and Sliding in Layered Materials: the Power of the Registry Index" – Invited Talk – "Recent Advances in Computational Modeling for Energy Applications", Haifa, Israel (July 7<sup>th</sup> 2015).

"Interlayer Commensurability and Sliding in Layered Materials: the Power of the Registry Index" – Invited Talk – "Advances in Modeling of Nano Materials" – a satellite meeting of the 15<sup>th</sup> International Congress of Quantum Chemistry (ICQC 2015), Hefei, China (June 15<sup>th</sup> 2015).

"A State Representation Approach for Atomistic Time-Dependent Transport Calculations in Molecular Junctions" – Invited Talk – The Batsheva de Rothschild Seminar on Molecular Electronics 2015 – 40 Year Later, Maale Hachamisha, Israel (June 8<sup>th</sup> 2015).

Co-organizer (together with Prof. Leeor Kronik) of the 2015 Symposium of the Lise Meitner – Minerva Center for Computational Quantum Chemistry, Tel Aviv University, Tel Aviv, Israel (May 3<sup>rd</sup> 2015).

"Interlayer Commensurability and Sliding in Layered Materials: the Power of the Registry Index" – Invited Talk – 249<sup>th</sup> National Meeting of the American Chemical Society, Denver, Colorado, USA (March 25<sup>th</sup> 2015).

"A State Representation Approach for Atomistic Time-Dependent Transport Calculations in Molecular Junctions" – Invited Talk – The First Northwestern University Tel Aviv University Workshop, Tel-Aviv, Israel (February 23<sup>rd</sup> 2015).

"A State Representation Approach for Atomistic Time-Dependent Transport Calculations in Molecular Junctions" – Invited Talk – The 80<sup>th</sup> Annual Meeting of the Israel Chemical Society, Tel-Aviv, Israel (February 19<sup>th</sup> 2015).

"A State Representation Approach for Atomistic Time-Dependent Transport Calculations in Molecular Junctions" – Invited Talk – Mini-Symposium on Electronic Structure and Dynamics, Weizmann Institute of Science, Rehovot, Israel (December 29<sup>th</sup> 2014).

"Interlayer Commensurability and Sliding in Layered Materials: the Power of the Registry Index" – Invited Talk – CECAM workshop on "Friction and Interface Dynamics at the Nano- and Mesoscales", Tel-Aviv University, Tel-Aviv, Israel (October 30<sup>th</sup> 2014).

"A State Representation Approach for Atomistic Time-Dependent Transport Calculations in Molecular Junctions" – Invited Talk – CECAM workshop on "High performance models of charge transport in large scale systems", University of Bremen, Bremen, Germany (October 7<sup>th</sup> 2014).

"A State Representation Approach for Atomistic Time-Dependent Transport Calculations in Molecular Junctions" – Invited Talk – The Isaiah Shavitt Workshop Series on: "Quantum Mechanics in Chemistry: From Structure to Dynamics" – Quantum Dynamics Day, Technion, Haifa, Israel (May 15<sup>th</sup> 2014).

"A State Representation Approach for Atomistic Time-Dependent Transport Calculations in Molecular Junctions" – Israel CECAM Flagship Workshop on "Quantum Dynamics in Molecular and Nano-Materials: Mechanisms and Functionality", Tel-Aviv University, Tel-Aviv, Israel (November 29<sup>th</sup> 2013).

Co-organizer (together with Prof. Eran Rabani) of the first Israel CECAM Flagship Workshop on "Quantum Dynamics in Molecular and Nano-Materials: Mechanisms and Functionality", Tel-Aviv University, Tel-Aviv, Israel (November 28<sup>th</sup> - December 1<sup>st</sup> 2013).

Co-organizer (together with Prof. Leeor Kronik) of the 2013 Symposium of the Lise Meitner - Minerva Center for Computational Quantum Chemistry, Weizmann Institute of Science, Rehovot, Israel (November 3<sup>rd</sup> 2013).

"Towards Graphene Based Ultrasensitive Chemical Detectors: Lithium Anchoring of Organic Molecules on the Surface of Graphene" – Invited Talk – International Conference on Electromagnetics in Advanced Applications, Torino, Italy (September 10<sup>th</sup> 2013).

"A State Representation Approach for Atomistic Time-Dependent Transport Calculations in Molecular Junctions" – Invited Talk – TSRC workshop on Quantum Transport in Nanoscale Molecular Systems, Telluride, Colorado, USA (July 9<sup>th</sup> 2013).

"Electronic Structure and Processes at Molecular-Based Interfaces" (ESPMI VII) - session chair on Photovoltaics – Weizmann Institute of Science, Rehovot, Israel (May 1<sup>st</sup> 2013).

"Interlayer Commensurability and Sliding in Layered Materials: the Power of the Registry Index" – Invited Talk – TAU-Tsinghua workshop on Nanoscience and Nanotechnology, Tel-Aviv University, Tel-Aviv, Israel (April 30<sup>th</sup> 2013).

"Interlayer Commensurability and Sliding in Layered Materials: the Power of the Registry Index" – Invited Talk – 2013 EMN Spring Meeting, Walt Disney World Swan and Dolphin Resort, Orlando, Florida (April 10<sup>th</sup> 2013).

"Molecular Interferometers: Circular Currents and Magnetic Field Effects in Molecular Rings" – Invited Talk – 78<sup>th</sup> meeting of the Israel Chemical Society – Dan Panorama Hotel, Tel-Aviv, Israel (February 13<sup>th</sup> 2013).

"Molecular Interferometers: Circular Currents and Magnetic Field Effects in Molecular Rings" – Invited Talk – Joint International Conference of the Israel Institute for Advanced Studies and the Israel Science Foundation on Molecular Electronics – Hebrew University, Jerusalem, Israel (July 16<sup>th</sup> 2012).

2012 MRS Spring Meeting & Exhibit – symposium co-organizer and session chair – "Computational Materials Design in Heterogeneous Systems", San Francisco, California, USA (April 9<sup>th</sup> -13<sup>th</sup> 2012).

"Interlayer Commensurability and Sliding in Layered Materials: the Power of the Registry Index" – Invited Talk - the Lise Meitner-Minerva Computational Chemistry Symposium, Hebrew University, Jerusalem, Israel (March 11<sup>th</sup> 2012).

"The Wonders of Graphene" – Invited Talk – 2010 Nobel prize seminar, The Open University of Israel, Raanana, Israel (May 18<sup>th</sup> 2011).

"The Wonders of Graphene" – Invited Talk – The 12<sup>th</sup> Asian Physics Olympiad , Kfar Hamaccabiah, Ramat-Gan, Israel (May 2<sup>nd</sup> 2011).

"Stacking and Registry Effects in Layered Materials: the Case of Hexagonal Boron-Nitride and beyond" – Invited Talk – Electrochemistry seminar, Tel-Aviv University, Tel-Aviv, Israel (April 13<sup>th</sup> 2011).

"Stacking and Registry Effects in Layered Materials: the Case of Hexagonal Boron-Nitride and beyond" – Invited Talk – CECAM workshop on charge and spin transport in chemically modified graphene based materials, Universitat Autònoma de Barcelona Bellaterra, Barcelona, Spain (April 8<sup>th</sup> 2011).

"Stacking and Registry Effects in Layered Materials: the Case of Hexagonal Boron-Nitride and beyond" – Invited Talk – The Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA, USA (March 29<sup>th</sup> 2011).

"Stacking and Registry Effects in Layered Materials: the Case of Hexagonal Boron-Nitride and beyond" – Invited Talk – US-India-Israel Workshop on Nanoscale Phenomena in Soft and Hybrid Matter, Northwestern University, Evanston, IL, USA (March 25<sup>th</sup> 2011).

"Stacking and Registry Effects in Layered Materials: the Case of Hexagonal Boron-Nitride" – Invited Talk – IVS symposium on "Carbon Nanostructures – from fundamentals to applications", Technion, Haifa, Israel (January 13<sup>th</sup> 2011).

"Stacking and Registry Effects in Layered Materials: the Case of Hexagonal Boron-Nitride" – Invited Talk – Tel-Aviv University's Physics Colloquium, Tel-Aviv, Israel (January 2<sup>nd</sup> 2011).

"The wonders of graphene" – Invited Talk – the National annual junior high-school science teachers meeting, Weizmann Institute of Science, Rehovot, Israel (December 8<sup>th</sup> 2010).



"The wonders of graphene" – Invited Talk – the National annual high-school chemistry teachers meeting, Rehovot, Weizmann Institute of Science, Israel (December 6<sup>th</sup> 2010).

"Stacking and Registry Effects in Layered Materials: the Case of Hexagonal Boron-Nitride" – Invited Talk – the Lise Meitner-Minerva Computational Chemistry Symposium, Hebrew University, Jerusalem, Israel (November 22<sup>th</sup> 2010).

"Stacking and Registry Effects in Hexagonal Boron-Nitride" – Invited Talk – Chemical Physics lunch club at the Weizmann Institute of Science, Rehovot, Israel (November 14<sup>th</sup> 2010).

"Stacking and Registry Effects in Layered Materials: The Case of Hexagonal Boron Nitride" - poster presentation -  $\psi_k$  ab-initio conference, Freie Universität, Berlin, Germany (September 13<sup>th</sup> 2010).

Co-organizer (together with prof. Yoram Selzer) of the Tel-Aviv Symposium in Chemical Physics: Focus on Electronic Transport in Molecular Junctions, Tel-Aviv University, Tel-Aviv, Israel (June 14<sup>th</sup> 2010).

"Stacking and Registry Effects in Hexagonal Boron-Nitride" – Invited Talk – Transition Metal Chalcogenide and Halide Nanostructures workshop at the Weizmann Institute of Science, Rehovot, Israel (April 26<sup>th</sup> 2010).

"Stacking and Registry Effects in Hexagonal Boron-Nitride" – Invited Talk – Nano Seminar at the Hebrew University, Jerusalem, Israel (April 11<sup>th</sup> 2010).

Session chair and member of the Scientific Committee, Tel-Aviv University Workshop on Nanoscience and Nanotechnology, Maalot, Israel (February 11<sup>th</sup> 2010).

"Stacking and Registry Effects in Hexagonal Boron-Nitride" – The 75<sup>th</sup> Meeting of the Israel Chemical Society, Tel-Aviv, Israel (January 25<sup>th</sup> 2010).

"Electro-Mechanical Properties of Boron-Nitride Nanotubes" – Invited Talk – MAFAT/AFRL Meta- and Bio/Nano Materials Workshop, Tel-Aviv University, Tel-Aviv, Israel (November 4<sup>th</sup> 2009).

Session Chair, Graphitic Materials Symposium, ACS Fall Meeting, Washington D.C., USA (August 19<sup>th</sup> 2009).

"Electro-Mechanical Properties of Suspended Graphene Nanoribbons" – Invited Talk – ACS Fall Meeting, Washington D.C., USA (August 16<sup>th</sup> 2009).

"Electro-Mechanical Properties of Suspended Graphene Nanoribbons" – Invited Talk – Physics Department Seminar, Central Michigan University, Mt. Pleasant, Michigan, USA (August 14<sup>th</sup> 2009).

"Electro-Mechanical Properties of Suspended Graphene Nanoribbons" – Invited Talk – The Annual Memorial Ceremony for the Late Prof. Y. M. Goldschmidt, Faculty of Exact Sciences, Department of Chemistry, Bar-Ilan University, Ramat-Gan, Israel (June 17<sup>th</sup> 2009).

"Electro-Mechanical Properties of Suspended Graphene Nanoribbons" – Invited Talk – 2nd Workshop on Computational Nanotechnology at the Technion, Haifa, Israel (April 22<sup>nd</sup> 2009).

"Electro-Mechanical Properties of Suspended Graphene Nanoribbons" – Invited Talk – Solid Mechanics and Systems Seminar at Tel-Aviv University, Tel-Aviv, Israel (March 23<sup>rd</sup> 2009).

"Electro-Mechanical Properties of Suspended Graphene Nanoribbons" – Invited Talk – Materials and Nano Seminar at Tel-Aviv University, Tel-Aviv, Israel (March 8<sup>th</sup> 2009).

"Electro-Mechanical Properties of Suspended Graphene Nanoribbons" – Invited Talk – The 5<sup>th</sup> workshop of the Center for Nanoscience & Nanotechnology at Tel-Aviv University, Ha'Goshrim, Israel (February 23<sup>rd</sup> 2009).

"Electro-Mechanical Properties of Suspended Graphene Nanoribbons" – Invited Talk – The 74<sup>th</sup> Meeting of the Israel Chemical Society, Tel-Aviv, Israel (February 8<sup>th</sup> 2009).

"Spin Dynamics in Graphene Molecular Derivatives" – Invited Talk – The Minerva Gentner Symposium on: Time Dependent Density Functional Theory, Eilat, Israel (2007).

"Graphene Nanoribbons – New Players in the Field of Nanoelectronics" – Invited Talk – Air Force Research Laboratory, Wright-Patterson Air Force Base, Dayton, Ohio, USA (2007).

"First-Principles Electronic Transport Calculations in Finite Elongated Systems: A Divide and Conquer Approach" – poster presentation – American Physical Society March Meeting – Denver, Colorado, USA (2007).

"Graphene Nanoribbons – New Players in the Field of Nanoelectronics" – oral presentation – University of Houston, Houston, Texas, USA (2007).

"Graphene Nanoribbons – New Players in the Field of Nanoelectronics" – oral presentation – Weizmann Institute of Science, Rehovot, Israel (2007).

"Graphene Nanoribbons – New Players in the Field of Nanoelectronics" – oral presentation – Hebrew University of Jerusalem, Jerusalem, Israel (2007).

"Graphene Nanoribbons – New Players in the Field of Nanoelectronics" – oral presentation – Technion – Israel Institute of Technology, Haifa, Israel (2007).

"Graphene Nanoribbons – New Players in the Field of Nanoelectronics" – oral presentation – Tel-Aviv University, Tel-Aviv, Israel (2007).

"First-Principles Electronic Transport Calculations in Finite Elongated Systems: A Divide and Conquer Approach" – oral presentation – Rice Quantum Institute Twentieth Annual Research Colloquium – Houston, Texas, USA (2006).

"Feasible Nanometric Magnetoresistance Devices" – poster presentation – American Conference on Theoretical Chemistry (ACTC2005) – UCLA, Los-Angeles, USA (2005).

"Feasible Nanometric Magnetoresistance Devices" – poster presentation – Tel-Aviv University Workshop on Nanoscience and Nanotechnology – Maagan, Israel (2005).

"Feasible Nanometric Magnetoresistance Devices" – oral presentation – Tel-Aviv University Workshop on Nanoscience and Nanotechnology – Kfar Bloom, Israel (2004).

"Molecular Nanopumps – A Coarse Grain Model" & "Feasible Nanometric Magnetoresistance Devices" – poster presentation – ICS meeting – Tel-Aviv, Israel (2003).

"Molecular Nanopumps – A Coarse Grain Model" – poster presentation – GRC conference on Clusters, Nanocrystals and Nanostructures – Connecticut, U.S.A. (2003).

"Molecular Nanopumps – A Coarse Grain Model" – poster presentation – Science and applications of Nanostructures – Jerusalem, Israel (2003).

"Closed Cage Carbon Nanotube Structures – Towards Nanoelectromagnets" – poster presentation – TheoChem 2002 symposium – Jerusalem, Israel (2002).

"Closed Cage Carbon Nanotube Structures – Towards Nanoelectromagnets" – poster presentation – Gentner symposium – Potsdam, Germany (2002).

Nobel laureates – students meeting – Lindau, Germany (2002).

"Closed Cage Carbon Nanotube Structures – Towards Nanoelectromagnets" – poster presentation – Lise Meitner Symposium on Quantum Chemistry – Jerusalem, Israel (2001).

**Military  
Service**

Years	Service
1998-2000	Israeli M.O.D.
1994-1998	I.D.F. – Air Force
Rank:	Major

**Extracurricular  
Activities**

1994-2009: Member of the Shotokan Karate-Do association in Israel (Dan-2).

2002-2005: Member of the Nisshin-Kan Aikido association in Israel (Q-5).

**Hobbies**

Spanish and acoustic Guitar.

Invited concerts performed on several stages playing Judeo-Espaniol Ladino Romances including:

- The world Jewish-Spanish Federation conference at the YMCA concert hall in Jerusalem.
- The 60 Years Jubilation of the Medical School and Hadassa Organization in the Hebrew University of Jerusalem at “Binyanei Hauma” concert hall in Jerusalem.