Dr. Amir Natan - Curriculum Vitae

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Date and Place of birth: April 6, 1966 , Ramat-Gan, Israel.
IDF military service: 7/84 till 7/92 (Talpiot project).
Marital status: Married.
No of children: 1

A. Education

1984-1987 – B.Sc. in Physics (wide) and Mathematics (wide), (Cum Laude) from the Hebrew University.
2003-2005 – M.Sc. in Electronics and Electrical Engineering (Cum Laude) from the Tel-Aviv University. Thesis: "Adsorption of benzene derivative self assembled monolayers on silicon surfaces: A first principles study", supervised by Prof. Y. Shapira and Dr. L. Kronik
2006-2010 – PhD at the Weizmann institute. Thesis "Understanding collective effects at organic/inorganic interfaces from first principles", supervised by Prof. L. Kronik and Prof. D. Cahen.

B. Further studies

October 2010- June 2011 – Post-doctorate fellowship in the group of Prof. Tamar Seideman at Northwestern University.

C. Academic and professional experience

1987-1988 – In Rafael on behalf of the Israeli Navy. Signal processing work.
1989-1992 – In the Israeli Air industries on behalf of the Israeli Navy. Signal processing consulting and algorithm development for a large scale project.
1992-1999 – Co-founder and President (1994-1997) of Compugen Ltd. (http://www.cgen.com, Nasdaq:cgen) together with 2 partners. The company still exists (2010) and has an affiliated company (Evogene Ltd.) in the area of plants genome analysis.
2003-2004 – Consultant for BrainsGate Ltd. - a company producing a medical device for the delivery of drugs across the blood-brain barrier.
2006,2009 – Teaching assistant, "Solid State Physics for Chemists" – Weizmann Institute, Israel.

October 2011 - Today – Senior Lecturer, Tel-Aviv University, Department of Physical Electronics. My group research areas: High Throughput Materials Science, Processes in photovoltaic cells and energy storage devices and light matter interaction. We use Density Functional Theory, Molecular Dynamics and also larger scale modeling for various physical problems. We also develop formalism and code for DFT and RT-TDDFT in the

real-space approach. My long term goal is to develop and use multi-scale methods to describe devices from atomic to macroscopic level.

Scientific publications

1. **Amir Natan**, Yigal Zidon, Yoram Shapira, and Leeor Kronik, "Cooperative effects and dipole formation at semiconductor/self-assembled-monolayer interfaces", Phys. Rev. B **73** 193310 (2006).
2. **Amir Natan**, Leeor Kronik and Yoram Shapira, "Computing surface dipoles and potentials of self-assembled monolayers from first principles", Applied Surface Science, **252,** 7608 (2006).
3. Rachel Gueta**, **Amir Natan****, Lia Addadi, Steve Weiner, Keith Refson, and Leeor Kronik, "Local atomic order and infrared spectra of biogenic calcite", Angewandte Chemie Int'l Edition, **46**, 291-294 (2007). **Equal contribution authors.
4. Lior Segev, Adi Salomon, **Amir Natan**, David Cahen, Leeor Kronik, Fabrice Amy, Calvin K. Chan, and Antoine Kahn, "Electronic structure of Si(111)-bound alkyl monolayers: Theory and experiment", Phys. Rev. B. **74**, 165323 (2006).
5. Rachela Popovtzer, **Amir Natan**, Yosi Shacham-Diamand, "Mathematical Model of Whole Cell Electrochemical Biosensor for Water Toxicity Detection", Journal of Electroanalytical Chemistry 206, 17 (2007).
6. **Amir Natan**, Leeor Kronik, Hossam Haick, and Raymond Tung, "Electrostatic properties of ideal and non-ideal polar organic monolayers: implications for electronic devices", Adv. Mat. **19**, *4103-4117,* (2007).
7. Dudi Deutsch, **Amir Natan**, Yoram Shapira, and Leeor Kronik, "Electrostatic properties of adsorbed polar molecules: Opposite behavior of a single molecule and a molecular monolayer", J. Am. Chem. Soc. 129, 2989 (2007).
8. **Amir Natan**, Ayelet Benjamini, Doron Naveh, Leeor Kronik, Murilo L. Tiago, Scott P. Beckman,and James R. Chelikowsky, "Real Space Pseudopotential method for first principles calculations of general periodic and partially periodic systems", Phys. Rev. B **78**, 075109 (2008).
9. Eyal Capua, **Amir Natan**, Leeor Kronik, and Ron Naaman, "The Molecularly Controlled Semiconductor Resistor: How does it work?", Appl. Mater. Interfaces, **1** (11), pp 2679–2683 (2009).
10. **Amir Natan,** Natalia Kuritz, and Leeor Kronik, "Polarizability, susceptibility, and dielectric constant of nano-scale molecular films: a microscopic view" – Adv. Func. Mater. **20**, 2077–2084 (2010).
11. Ferdinand Rissner, David A. Egger, **Amir Natan**, Thomas Körzdörfer, Stephan Kümmel, Leeor Kronik, and Egbert Zojer, "Collectively Induced Quantum-Confined Stark Effect in Monolayers of Molecules Consisting of Polar Repeating Units", JACS **133**, 18634-18645 (2011).
12. Ferdinand Rissner, **Amir Natan**, David A. Egger, Oliver T. Hofmann, Leeor Kronik and Egbert Zojer, "Dimensionality effects in the electronic structure of organic semiconductors consisting of polar repeat units", Organic Electronics, **13** , 3165 (2012).

13. **Amir Natan**, Mark C. Hersam and Tamar Seideman**,** "Insights into graphene functionalization by single atom doping"**,** IOP Nanotechnology **24**, 505715 (2013).
14. Nadav Amdursky, Gil Shalev, Amir Handelman, Simon Litsyn, **Amir Natan**, Yakov Roizin, Yossi Rosenwaks, Daniel Szwarcman, Gil Rosenman **,** "Bioorganic nanodots for non-volatile memory devices"**,** APL MATERIALS **1**, 062104 (2013).
15. Yevgeny Rakita, Diana Golodnitsky, **Amir Natan**, "Electrostatic potential of polyelectrolyte molecules grafted on charged surfaces: A Poisson-Boltzmann model", Journal of Electrochemical Society **161** (8), E3049-E3058, (2014).
16. Amir Handelman, **Amir Natan**, Gil Rosenman, "Structural and optical properties of short peptides: nanotubes-to-nanofibers phase transformation", Journal of Peptide Science (2014).
17. **Amir Natan**, Fock-Exchange for periodic structures in the real-space formalism and the KLI approximation", PCCP, **17**, 31510 (2015), DOI: 10.1039/C5CP01093D.
18. M. Zuzovski, A. Boag and **A. Natan**, "Auxiliary grid method for the calculation of electrostatic terms in Density Functional Theory on a real-space grid", PCCP, **17**, 31510, (2015).
19. Camilo E. Calderon, Jose J. Plata, Cormac Toher, Corey Oses, Ohad Levy, Marco Fornari, **Amir Natan**, Michael J. Mehl, Gus Hart, Marco Buongiorno Nardelli, Stefano Curtarolo, "The AFLOW Standard for High-Throughput Materials Science Calculations", Computational Materials Science (IF 2.1), Computational Materials Science **108** (2015) 233–238.
20. Amir Handelman, Natalia Kuritz, **Amir Natan** and Gil Rosenman, "Reconstructive Phase Transition in Ultrashort Peptide Nanostructures and Induced Visible Photoluminescence", Langmuir **32**, 2847 (2016). DOI: 10.1021/acs.langmuir.5b02784.
21. Nicholas Boffi, Manish Jain and **Amir Natan**, "Asymptotic behavior and interpretation of virtual states: the effects of confinement and of basis sets" – J. Chem. Phys. **144**, 084104 (2016).
22. Natalia Kuritz, Michael Murat, Moran Balaish, Yair Ein-Eli, and **Amir Natan**, "PFC and Triglyme for Li-Air Batteries: A Molecular Dynamics Study" – J. Phys. Chem. B **120** (13), pp 3370–3377 (2016). DOI: 10.1021/acs.jpcb.5b12075.
23. Christopher M. Caskey, Aaron Holder, Sarah Shulda, Steve Christensen, David Diercks, Craig P. Schwartz, David Biagioni, Dennis Nordlund, Chilan Ngo, Alon Kukliansky, **Amir Natan**, Bernado Orvananos, Xuiwen Zhang, Gerbrand Ceder, David Prendergast, David S. Ginley, John D. Perkins, Suneel Kodambaka, Vladan Stevanovic, Svitlana Pylypenko, Stephan Lany, Ryan M. Richards, Andriy Zakutayev, "Synthesis of a mixed-valent tin nitride and considerations of its possible crystal structures" – J. Chem. Phys. **144**, 144201 (2016).
24. Nicholas Boffi, Manish Jain and **Amir Natan**, "Efficient computation of the Hartree-Fock exchange in real-space with projection operators" – JCTC **12**, 3614 (2016), DOI:10.1021/acs.jctc.6b00376.

25. Dor Gabay, Amir Boag, and **Amir Natan**, "Optimizing kernel methods for Poisson integrals on a uniform grid" – Computer Physics Communications (CPC) **215**, 1-6 (2017), DOI: 10.1016/j.cpc.2017.01.016. Citations 1/0, IF: 3.9, LEVEL: Q1 (Hardware and Architecture; Physics and Astronomy – misc.).
26. Dor Gabay, Xueyang Wang, Vitaly Lomakin, Amir Boag, Manish Jain and **Amir Natan** "Size dependent electronic properties of silicon quantum dots - an analysis with hybrid, screened hybrid and local density functional theory", Computer Physics Communications (CPC) **221**, 95-101 (2017), DOI: 10.1016/j.cpc.2017.08.005.
27. Faktorovich-Simon E., **A. Natan**, E. Peled, and D. Golodnitsky, "Oxygen redox processes in PEGDME-based electrolytes for the Na-air battery." Journal of Solid State Electrochemistry (2017): 1-8.
28. Alon Hever, Corey Oses, Stefano Curtarolo, Ohad Levy, and **Amir Natan**, "The structure and composition statistics of 6A binary and ternary crystalline materials" – ACS Inorganic Chemistry (2017) , DOI: 10.1021/acs.inorgchem.7b02462.
29. Keren Raz, Polina Tereshchuk, Diana Golodnitsky, and **Amir Natan**, "Adsorption of Li2O2, Na2O2 and NaO2 on TiC(111) Surface for Metal-Air Rechargeable Batteries: A Theoretical Study", Journal of Physical Chemistry C (2018), DOI: 10.1021/acs.jpcc.8b01983.
30. Natalia Kuritz, Goren Gordon, and **Amir Natan**, "Size and Temperature Transferability of Direct and Local Deep Neural Networks for Atomic Forces", Phys. Rev. B **98**, 094109 (2018).
31. Adrian Schürmann, Ronja Haas, Michael Murat, Natalia Kuritz, Moran Balaish, Yair Ein-Eli, Juergen Janek, **Amir Natan****, Daniel Schröder**, "Diffusivity and Solubility of Oxygen in Solvents for Metal/Oxygen Batteries: A Combined Theoretical and Experimental Study", the Journal of Electrochemical Society (JES) **165** (13) A3095-A3099 (2018), DOI: 10.1149/2.0601813jes . **Equal corresponding authors.
32. Eldad Yahel and **Amir Natan**, "Effect of multiorbital contributions to strong-field ionization of benzene derivatives", Phys. Rev. A **98**, 053421 (2018).
33. Nadezda Lapshina, Ivan I. Shishkin, Ramesh Nandi, Roman E. Noskov, Hani Barhom, Sijo Joseph, Boris Apter, Tal Ellenbogen, **Amir Natan**, Pavel Ginzburg, Nadav Amdursky, Gil Rosenman, *Advanced Optical Materials (2018). DOI: 10.1002/adom.201801400.*
34. Sijo K. Joseph, Natalia Kuritz, Eldad Yahel, Nadezda Lapshina, Gil Rosenman and **Amir Natan**, "Proton-Transfer Induced Fluorescence in Self Assembled Short Peptides", Journal of Physical Chemistry A, **123** (9), 1758-1765 (2019). DOI: 10.1021/acs.jpca.8b09183.
35. Evelina Faktorovich-Simon, **Amir Natan**, Emanuel Peled, and Diana Golodnitsky, "Comparison of the Catalytic Activity of Carbon, Spinel-Based, and Carbide Materials in the Na-Air Battery", Frontiers of Materials, **6**, 249, (2019), DOI: 10.3389/fmats.2019.00249.
36. Mivsam Yekutiel, Alon Kukliansky, and **Amir Natan**, "Cu2MgO3 electronic and magnetic properties - a DFT study", accepted for publication in the Israel Journal of Chemistry. DOI: 10.1002/ijch.201900100.

37. Eliran Hamo, Polina Tereshchuk, Melina Zysler, David Zitoun, **Amir Natan**, and Brian A. Rosen "Corrosion resistance and acidic ORR activity of Pt-based catalysts supported on nanocrystalline alloys of molybdenum and tantalum carbide", Journal of Electrochemical Society (JES) **166** (16), F1292-F1300 (2019).

Conference papers:

1. Viktor Ariel and **Amir Natan**, "Electron effective mass in graphene", International Conference on Electromagnetics in Advanced Applications *(ICEAA), 2013*, vol., no., pp.696,698, 9-13 Sept. 2013 , doi: 10.1109/ICEAA.2013.6632334.

2. **A. Natan**, M. Zuzovski, A. Boag, G. Slepyan, P. Ramsamy, P. Poullet, "Fock Exchange: optimization challenges on a real-space grid" – International Conference on Electromagnetics in Advanced Applications *(ICEAA), 2014.*

3. M. Zuzovski, A. Boag, G. Slepyan, P. Poullet, **A. Natan**, "Calculation of Elongated Carbon Structures with Density Functional Theory and Fast Poisson Solver" - International Conference on Electromagnetics in Advanced Applications *(ICEAA), 2015.*

4. A Boag, **A Natan**, P Poullet, G Slepyan, "Edge states and edge conditions for electromagnetic field in nanophotonics" - International Conference on Electromagnetics in Advanced Applications *(ICEAA), 2015.*

5. E. Segev and **Amir Natan**, "Effects of multiple atom doping in graphene", - International Conference on Electromagnetics in Advanced Applications *(ICEAA), 2017.*