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Curriculum Vitae - Noa Marom

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Education:

2004-2010 Weizmann Institute of Science
Ph.D. (direct track), Department of Materials and Interfaces, Faculty of Chemistry
Thesis: *A first principles description of the electronic structure of organic semiconductors*
Advisor: Leeor Kronik
1998- 2003 Technion - Israel Institute of Technology
B.Sc., *Cum Laude*, Materials Engineering
B.A., *Cum Laude*, Physics
2000- 2001 University of Pittsburgh, Pittsburgh, PA (via student exchange)

Academic Positions:

2025- Professor, Materials Science and Engineering, Carnegie Mellon University
2025- Courtesy Professor, Department of Chemistry and Department of Physics, Carnegie Mellon University
2025- Adjunct Professor, Department of Physics & Astronomy, the University of Pittsburgh
2021-2025 Associate Professor, Materials Science and Engineering, Carnegie Mellon University
2021-2025 Courtesy Associate Professor, Department of Chemistry and Department of Physics, Carnegie Mellon University
2023-2025 Adjunct Associate Professor, Department of Physics & Astronomy, the University of Pittsburgh
2016-2021 Assistant Professor, Materials Science and Engineering, Carnegie Mellon University
2016-2021 Courtesy Assistant Professor, Department of Chemistry and Department of Physics, Carnegie Mellon University
2013-2016 Assistant Professor, Physics and Engineering Physics, Tulane University
2010-2013 Postdoctoral Fellow, Institute for Computational Engineering and Sciences (ICES), The University of Texas at Austin; Advisor: James R. Chelikowsky

Other Employment History:

2002- 2004 Application Engineer, Applied Materials, Rehovoth, Israel
2001- 2002 Undergraduate Research Assistant, Physics Department, Technion
1996-1998 Military Service, IDF Communications Corps (honorably discharged, last rank: Sergeant)

Awards:

- Award for Best Presentation, *The 14th Israel Materials Engineering Conference (IMEC-14)*, Tel-Aviv, Israel, 12/09.
- Minerva Short-Term Research Grant to Germany, 2010.
- **The Shimon Reich Memorial Prize of Excellence** of the Feinberg Graduate School of the Weizmann Institute of Science, 2010.
- The Materials Computation Center (MCC) Travel Award to attend the Psi-K Conference, 2010.
- The DOE Advanced Scientific Computing Research (ASCR) Leadership Computing Challenge (ALCC) Award for "Toward Crystal Engineering from First Principles", 2011 (co-PI).

- The Materials Computation Center (MCC) Travel Award to attend the conference “Towards First-Principles Description of van der Waals Interactions in Complex Materials”, 2012.
- The DOE Advanced Scientific Computing Research (ASCR) Leadership Computing Challenge (ALCC) Award for “Interfaces in Organic and Hybrid Photovoltaics”, 2014.
- The Tulane Committee on Research (COR) Faculty International Travel Grant to attend the European Materials Research Society (E-MRS) 2014 Spring Meeting, 2014.
- The Materials Computation Center (MCC) Travel Award to attend the conference “Addressing Challenges for First-Principles Based Modeling of Molecular Materials”, 2014.
- The Louisiana Board of Regents (BoR) Travel Grant for Emerging Faculty (TGEF) to attend the ACS National Meeting, 2015.
- The DOE Advanced Scientific Computing Research (ASCR) Leadership Computing Challenge (ALCC) Award for “Computational Design of Interfaces for Photovoltaics”, 2015.
- The Tulane Committee on Research (COR) Faculty International Travel Grant to attend the Theory of Metal Atoms, Clusters and Nanoparticles Stabilized by Organic Matter Workshop in Helsinki, Finland, 2015.
- **The Sanibel Symposium Young Investigator Award**, 2016
- **NSF CAREER Award** for “Structure Prediction and Design of Molecular Crystals with the Gator Genetic Algorithm Package”, 2016-2021.
- **DOE Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Award** for “Materials and Interfaces for Organic and Hybrid Photovoltaics”, 2017.
- **The Charles E. Kaufman New Investigator grant**, 2017-2019.
- **DOE Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Award** for “Materials and Interfaces for Organic and Hybrid Photovoltaics”, 2018.
- **August-Wilhelm Scheer Visiting Professorship**, Technical University of Munich, 2018
- **The IUPAP Young Scientist Prize in Computational Physics**, 2018
- **DOE Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Award** for “Materials and Interfaces for Organic and Hybrid Photovoltaics”, 2019
- **Aurora Early Science Program (ESP) data and learning project** (2019-2025)
- The DOE Advanced Scientific Computing Research (ASCR) Leadership Computing Challenge (ALCC) Award for “Many-Body Perturbation Theory Meets Machine Learning to Discover Materials for Organic Photovoltaics”, 2020
- The George Tallman Ladd Award of the CMU College of Engineering, 2020
- **The ACS COMP OpenEye Outstanding Junior Faculty Award**, 2021
- CMU College of Engineering Dean’s Early Career Fellowship, 2021
- **Fellow of the American Physical Society**, 2025
- **DOE Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Award** for “Predicting excited-states of organic semiconductor crystals with GW+BSE and ML”, 2026

Publications in Peer-Reviewed Journals:

Total: 88 published, 6 submitted

High impact publications: 3 PRL; 1 Angew. Chem.; 2 JPCL; 6 PRB Rapid; 1 JMCC; 2 npj Comp. Mater.; 1 Chem. Mater.; 2 ACS AMI; 1 ACS Central Science; 1 ACS Nano.

Google Scholar h-index: 36; i10 index: 79; >6100 citations as of 8/25/26

- 1) 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).
- 2) N. Marom and L. Kronik, “*Density Functional Theory of Transition Metal Phthalocyanines. I: Electronic Structure of NiPc and CoPc - Self-Interaction Effects*”, *Appl. Phys. A* **95** 159 (2009) (Invited paper, special issue on Organic Materials for Electronic Applications).
- 3) N. Marom and L. Kronik, “*Density Functional Theory of Transition Metal Phthalocyanines. II: Electronic Structure of MnPc and FePc – Symmetry and Symmetry Breaking*”, *Appl. Phys. A* **95** 165 (2009) (Invited paper, special issue on Organic Materials for Electronic Applications).
- 4) T. Körzdörfer, S. Kümmel, N. Marom, and L. Kronik, “*When to Trust Photoelectron Spectra from Kohn-Sham Eigenvalues: The Case of Organic Semiconductors*”, *Phys. Rev. B* **79** 201205(R) (2009); *Phys. Rev. B* **82** 129903 (2010) (E).

- 5) B. D. Schultz, N. Marom, D. Naveh, X. Lou, C. Adelman, J. Strand, P. A. Crowell, L. Kronik, and C. J. Palmström, “*Spin Injection Across The Fe/GaAs Interface: Dominated by Interfacial Ordering*”, *Phys. Rev. B* **80** 201309(R) (2009).
- 6) N. Marom, A. Tkatchenko, M. Scheffler, and L. Kronik, “*A Balanced Description of Dispersive Interactions and Electronic Structure Using Density Functional Theory: The Case of Metal-Phthalocyanine Dimers*”, *J. Chem. Theory Comput.* **6** 81 (2010) [One of the top ten most-accessed articles in *Journal of Chemical Theory and Computation* in the first quarter of 2010].
- 7) N. Marom, J. Bernstein, J. Garel, A. Tkatchenko, E. Joselevich, L. Kronik, and O. Hod “*Stacking and Registry Effects in Layered Materials: The Case of Hexagonal Boron Nitride*”, *Phys. Rev. Lett.* **105** 046801 (2010).
- 8) N. Marom, A. Tkatchenko, S. Kapishnikov, L. Kronik, and L. Leiserowitz “*Structure and Formation of Synthetic Hemozin: Insights from First Principles Calculations*”, *Crystal Growth & Design* **11** 3332 (2011).
- 9) 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 (2011).
- 10) N. Marom, X. Ren, J. E. Moussa, J. R. Chelikowsky, and L. Kronik “*Electronic Structure of Copper Phthalocyanine from G_0W_0 Calculations*”, *Phys. Rev. B* **84**, 195143 (2011).
- 11) N. Marom, J. E. Moussa, X. Ren, A. Tkatchenko, and J. R. Chelikowsky “*Electronic Structure of Dye-Sensitized TiO_2 Clusters from Many-Body Perturbation Theory*”, *Phys. Rev. B* **84** 245115 (2011).
- 12) J. E. Moussa, N. Marom, N. Sai, and J. R. Chelikowsky “*Theoretical Design of a Shallow Donor in Diamond by Lithium-Nitrogen Codoping*”, *Phys. Rev. Lett.* **108** 226404 (2012).
- 13) N. Marom, M. Kim, and J. R. Chelikowsky “*Structure Selection Based on High Vertical Electron Affinity for TiO_2 Clusters*”, *Phys. Rev. Lett.* **108** 106801 (2012).
- 14) T. Körzdörfer and N. Marom “*A Strategy for Finding a Reliable Starting Point for G_0W_0 Demonstrated for Molecules*”, *Phys. Rev. B* **86** 041110(R) (2012).
- 15) T. Körzdörfer, R. M. Parrish, N. Marom, J. S. Sears, C. D. Sherrill, and J. L. Brédas “*Assessment of the Performance of Tuned Range-Separated Hybrid Density Functionals in Predicting Accurate Quasiparticle Spectra*”, *Phys. Rev. B* **86** 205110 (2012).
- 16) N. Marom, F. Caruso, X. Ren, O. Hofmann, T. Körzdörfer, J. R. Chelikowsky, A. Rubio, M. Scheffler, and P. Rinke “*Benchmark of GW Methods for Azabenzenes*”, *Phys. Rev. B* **86** 245127 (2012).
- 17) E. Salomon, P. Amsalem, N. Marom, L. Kronik, N. Koch, and T. Angot “*Electronic Structure of CoPc Adsorbed onto Ag(111): Evidence for Molecule-Substrate Interaction Mediated by Co 3d Orbitals*”, *Phys. Rev. B* **87** 075407 (2013).
- 18) B. Schatschneider, J. Liang, A. M. Reilly, N. Marom, G. Zhang, and A. Tkatchenko “*Electrodynamic Response and Stability of Molecular Crystals*”, *Phys. Rev. B* **87** 060104(R) (2013).
- 19) N. Marom, R. A. DiStasio Jr., V. Atalla, S. Levchenko, A. M. Reilly, J. R. Chelikowsky, L. Leiserowitz, and A. Tkatchenko “*Many-Body Dispersion Interactions in Molecular Crystal Polymorphism*”, *Angew. Chem. Int. Ed.* **52** 6629 (2013).
- 20) T. Straasø, N. Marom, I. Solomonov, L. K. Barfod, M. Burghammer, R. Feidenhans'l, J. Als-Nielsen, and L. Leiserowitz “*The Malaria Pigment Hemozin Comprises at Most Four Different Isomer Units in Two Crystalline Models: Chiral as Based on a Biochemical Hypothesis, or Centrosymmetric Made of Enantiomorphous Segments*”, *Crystal Growth & Design*, **14** 1543 (2014).
- 21) N. Marom, T. Körzdörfer, X. Ren, A. Tkatchenko, and J. R. Chelikowsky “*Size Effects in the Interface Level Alignment of Dye-Sensitized TiO_2 Clusters*”, *J. Phys. Chem. Lett.* **5** 2395 (2014).
- 22) N. S. Bobbitt, M. Kim, N. Sai, N. Marom, and J. R. Chelikowsky “*First Principles Calculations for Size Trends in Ga- and Al-Doped Zinc Oxide Nanocrystals with Wurtzite and Zincblende Structures*”, *J. Chem. Phys.*, **141** 094309 (2014).
- 23) M. Kim, N. Marom, N. S. Bobbitt, and J. R. Chelikowsky “*A First-Principles Study of the Electronic and Structural Properties of Sb and F doped SnO_2 Nanocrystals*”, *J. Chem. Phys.*, **142** 044704 (2015).

- 24) S. Bhattacharya, B. H. Sonin, C. J. Jumonville, L. M. Ghiringhelli, and N. Marom “Computational Design of Nanoclusters by Property-Based Genetic Algorithms: Tuning the Electronic Properties of $(\text{TiO}_2)_n$ Clusters”, *Phys. Rev. B* **91**, 241115(R) (2015).
- 25) X. Ren, N. Marom, F. Caruso, M. Scheffler, and P. Rinke “Beyond the GW Approximation: a Second-Order Screened Exchange Correction”, *Phys. Rev. B* **92**, 081104(R) (2015).
- 26) R. M. Richard, M. S. Marshall, O. Dolgounitcheva, J. V. Ortiz, J. L. Brédas, N. Marom, and C. D. Sherrill “Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules I: Reference Data at the CCSD(T) Complete Basis Set Limit”, *J. Chem. Theory Comput.* **12**, 595 (2016).
- 27) L. Gallandi, N. Marom, P. Rinke, and T. Körzdörfer “Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules II: Non-empirically Tuned Long-range Corrected Hybrid Functionals”, *J. Chem. Theory Comput.* **12**, 605 (2016).
- 28) J. Knight, X. Wang, L. Gallandi, O. Dolgounitcheva, X. Ren, J. V. Ortiz, P. Rinke, T. Körzdörfer, and N. Marom “Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules III: A Benchmark of GW Methods”, *J. Chem. Theory Comput.* **12**, 615 (2016).
- 29) O. Dolgounitcheva, M. Díaz-Tinoco, V. G. Zakrzewski, R. M. Richard, N. Marom, C. D. Sherrill, and J. V. Ortiz “Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules IV: Electron-Propagator Methods”, *J. Chem. Theory Comput.* **12**, 627 (2016); *ibid.* **13**, 389 (2017) (E).
- 30) A. M. Reilly et al. “Report on the Sixth Blind Test of Organic Crystal-Structure Prediction Methods”, *Acta Crystallographica B* **72**, 439 (2016).
- 31) F. Curtis, X. Wang, and N. Marom “Effect of Packing Motifs on the Energy Ranking and Electronic Properties of Putative Crystal Structures of Tricyano-1,4-dithiino[c]-isothiazole”, *Acta Crystallographica B* **72**, 562 (2016).
- 32) X. Wang, T. Garcia, S. Monaco, B. Schatschneider, and N. Marom “Effect of Crystal Packing on the Excitonic Properties of Rubrene Polymorphs”, *CrystEngComm*, **18**, 7353 (2016) (invited paper, special issue on Solid-State Photochemistry).
- 33) N. Marom “Accurate Description of the Electronic Structure of Organic Semiconductors by GW Methods”, *J. Phys.: Condens. Matter* **29**, 103003 (2017) (invited topical review).
- 34) A. Thierbach, C. Neiss, L. Gallandi, N. Marom, T. Körzdörfer, and A. Görling “Accurate valence ionization energies from Kohn-Sham eigenvalues with the help of potential adjustors”, *J. Chem. Theory Comput.*, **13**, 4726 (2017).
- 35) F. Curtis, X. Li, T. Rose, A. Vazquez-Mayagoitia, S. Bhattacharya, L. M. Ghiringhelli, and N. Marom “Gator: A First-Principles Genetic Algorithm for Molecular Crystal Structure Prediction”, *J. Chem. Theory Comput.*, **14**, 2246 (2018)
- 36) X. Li, F. Curtis, T. Rose, C. Schober, A. Vazquez-Mayagoitia, K. Reuter, H. Oberhofer, and N. Marom “Genarris: Random Generation of Molecular Crystal Structures and Fast Screening with a Harris Approximation”, *J. Chem. Phys.* **148**, 241701(2018) (invited paper, special issue on Data-Enabled Theoretical Chemistry).
- 37) X. Wang, X. Liu, C. J. Cook, B. Schatschneider, and N. Marom “On the Possibility of Singlet Fission in Crystalline Quaterylene”, *J. Chem. Phys.* **148** 184101 (2018).
- 38) F. Curtis, T. Rose, and N. Marom “Evolutionary Niching in the Gator Genetic Algorithm for Molecular Crystal Structure Prediction”, *Faraday Discussions* **211**, 61 (2018) (invited paper: themed collection on “Methods and applications of crystal structure prediction”).
- 39) M. Hammouri, T. Garcia, C. Cook, S. Monaco, S. Jezowski, N. Marom, and B. Schatschneider “Pressure Dependent High-throughput DFT Investigation of Herringbone Polycyclic Aromatic Hydrocarbons (HB-PAHs): Part 1. Pressure Dependent Structure Trends”, *J. Phys. Chem. C* **122**, 23815 (2018).
- 40) M. Hammouri, T. Garcia, C. Cook, S. Monaco, S. Jezowski, N. Marom, and B. Schatschneider “Pressure Dependent High-throughput DFT Investigation of Herringbone Polycyclic Aromatic Hydrocarbons (HB-PAHs): Part 2. Pressure Dependent Electronic Properties”, *J. Phys. Chem. C* **122**, 23828 (2018).
- 41) M. Addicoat et al. “Structure Searching Methods: General Discussion” *Faraday Discussions* **211**, 133 (2018)
- 42) M. Addicoat et al. “Crystal Structure Evaluation: Calculating Relative Stabilities and Other Criteria: General Discussion” *Faraday Discussions* **211**, 325 (2018)

- 43) X. Wang, X. Liu, R. Tom, C. J. Cook, B. Schatschneider, and N. Marom "Phenylated Acene Derivatives as Candidates for Intermolecular Singlet Fission", *J. Phys. Chem. C* **123**, 5890 (2019).
- 44) M. Yu, X. Wang, X. Du, C. Kunkel, T. Garcia, S. Monaco, B. Schatschneider, H. Oberhofer, and N. Marom "Anomalous Pressure Dependence of the Electronic Properties of Molecular Crystals Explained by Changes in Intermolecular Electronic Coupling", *Synthetic Metals*, **253**, 9 (2019) (invited paper, "Early Career Leaders" special issue).
- 45) R. Tom, T. Rose, I. Bier, H. O'Brien, A. Vazquez-Mayagoitia, and N. Marom "Genarris 2.0: A Random Structure Generator for Molecular Crystals", *Comput. Phys. Commun.*, **250**, 107170 (2020) (invited paper, "CPC 50th Anniversary" issue).
- 46) X. Liu, R. Tom, X. Wang, C. J. Cook, B. Schatschneider, and N. Marom "Pyrene-Stabilized Acenes as Intermolecular Singlet Fission Candidates: Importance of Exciton Wave-Function Convergence", *J. Phys.: Condens. Matter*, **32** 184001 (2020) (invited paper, "Emerging Leaders 2019" special issue).
- 47) S. Yang, C. Wu, and N. Marom "Topological Properties of SnSe/EuS and SnTe/CaTe Heterostructures", *Phys. Rev. Materials*, **4** 034203 (2020).
- 48) X. Wang, R. Tom, X. Liu, D. Congreve, and N. Marom "An Energetics Perspective on Why There Are So Few Triplet-Triplet Annihilation Emitters", *J. Mater. Chem. C*, **8**, 10816 (2020) (invited paper, "Emerging Investigators" themed issue; selected for the online collection highlighting the most popular articles published in Journal of Materials Chemistry C in 2020).
- 49) M. Yu, S. Yang, C. Wu, and N. Marom "Machine Learning the Hubbard U Parameter in DFT+U Using Bayesian Optimization", *npj Computational Materials* **6**, 180 (2020).
- 50) N. P. Zaitseva, A. M. Glenn, M. L. Carman, A. N. Mabe, S. A. Payne, N. Marom, X. Wang, "Multiple Dye Interactions in Plastic Scintillators: Effects on Pulse Shape Discrimination", *Nuclear Instruments and Methods in Physics Research A* **978**, 164455 (2020)
- 51) S. Yang, I. Bier, W. Wen, J. Zhan, S. Moayedpour, and N. Marom "Ogre: A Python Package for Molecular Crystal Surface Generation with Applications to Surface Energy and Crystal Habit Prediction", *J. Chem. Phys.* **152**, 244122 (2020) (invited paper, "2020 Emerging Investigators Collection").
- 52) X. Liu, R. Tom, S. Gao, and N. Marom "Assessing Zethrene Derivatives as Singlet Fission Candidates Based on Multiple Descriptors", *J. Phys. Chem. C* **124**, 26134 (2020) (invited paper, "Josef Michl Festschrift").
- 53) I. Bier and N. Marom "A Machine Learned Model for Solid Form Volume Estimation Based on Packing-Accessible Surface and Molecular Topological Fragments", *J. Phys. Chem. A* **124**, 10330 (2020).
- 54) M. Yu, S. Moayedpour, S. Yang, D. Dardzinski, C. Wu, V. S. Pribyl, N. Marom "Dependence of the Electronic Structure of the EuS/InAs Interface on the Bonding Configuration", *Phys. Rev. Mater.* **5**, 064606 (2021).
- 55) C. L. Hall, I. Andrusenko, J. Potticary, S. Gao, X. Liu, W. Schmidt, N. Marom, M. Gemmi, S. R. Hall "3D Electron Diffraction Structure Determination of Terrylene, a Promising Candidate for Intermolecular Singlet Fission", *ChemPhysChem*, **22**, 1631 (2021).
- 56) S. Moayedpour, D. Dardzinski, S. Yang, A. Hwang, N. Marom "Structure Prediction of Epitaxial Inorganic Interfaces by Lattice and Surface Matching with Ogre", *J. Chem. Phys.*, **155**, 034111 (2021) (invited paper, "Special Collection in Honor of Women in Chemical Physics and Physical Chemistry").
- 57) S. Yang, D. Dardzinski, A. Hwang, D. I. Pikulin, G. W. Winkler, N. Marom "First Principles Feasibility Assessment of a Topological Insulator at the InAs/GaSb Interface", *Phys. Rev. Mater.* **5**, 084204 (2021).
- 58) I. Bier, D. O'Connor, Y. T. Hsieh, W. Wen, A. M. Hiszpanski, T. Y. J. Han, N. Marom "Crystal Structure Prediction of Energetic Materials and a Twisted Arene with Genarris and Gator", *CrystEngComm*, **23**, 6023 (2021) (invited paper, "Computer-Aided Solid Form Design" themed collection; Selected for the CrystEngComm quarterly HOT article collection, featuring the top 10% of articles published in the journal each quarter).
- 59) S. Yang, N. Schröter, S. Schuwalow, M. Rajpalk, K. Ohtani, P. Krogstrup, G. W. Winkler, J. Gukelberger, D. Gresch, G. Aepli, V. N. Strocov, R. M. Lutchyn, N. Marom "Electronic Structure of InAs and InSb Surfaces: Density Functional Theory and Angle-Resolved Photoemission Spectroscopy" *Advanced Quantum Technologies*, **5**, 2100033 (2022) (Selected for the "Surfaces and Interfaces" Hot Topic)

- 60) D. Dardzinski, M. Yu, S. Moayedpour, and N. Marom “Best Practices for First-Principles Simulations of Epitaxial Inorganic Interfaces”, *J. Phys. Condensed Matter*, **34**, 233002 (2022) (Invited paper, Special Issue on “Women in Computational Condensed Matter Physics”)
- 61) X. Liu, X. Wang, S. Gao, V. Chang, R. Tom, M. Yu, L. M. Ghiringhelli, N. Marom “Finding Predictive Models for Singlet Fission by Machine Learning”, *npj Computational Materials*, **8**, 70 (2022).
- 62) X. Wang and N. Marom “An energetics assessment of benzo[a]tetracene and benzo[a]pyrene as triplet-triplet annihilation emitters”, *Molecular Systems Design & Engineering*, **7**, 889 (2022)
- 63) D. O’Connor, I. Bier, Y. T. Hsieh, N. Marom “Performance of Dispersion-Inclusive Density Functional Theory Methods for Energetic Materials”, *J. Chem. Theory Comput.* **18**, 4456 (2022)
- 64) X. Wang, S. Gao, M. Zhao, and N. Marom “Benchmarking time-dependent density functional theory for singlet excited states of thermally activated delayed fluorescence chromophores” *Phys. Rev. Research*, **4**, 033147 (2022).
- 65) S. Zelzer, R. Batabyal, D. Dardzinski, N. Marom, K. Grove-Rasmussen, P. Krogstrup “Scale-dependent optimized homoepitaxy of InAs(111)A”, *Cryst. Growth Des.* **22**, 5958 (2022)
- 66) I. Andrusenko, C. L. Hall, E. Mugnaioli, J. Potticary, S. R. Hall, W. Schmidt, S. Gao, K. Zhao, N. Marom, M. Gemmi “True molecular conformation and structure determination by three-dimensional electron diffraction of PAH by-products potentially useful for electronic applications”, *IUCrJ* **10**, 131 (2023)
- 67) B. Heischmidt, M. Yu, D. Dardzinski, J. Etheridge, S. Moayedpour, V. S. Pribyag, P. A. Crowell, N. Marom “First Principles Study of the Electronic Structure of the Ni₂MnIn/InAs and Ti₂MnIn/InSb Interfaces”, *Phys. Rev. Materials*, **7**, 026203 (2023)
- 68) R. Tom, S. Gao, Y. Yang, K. Zhao, I. Bier, E. A. Buchanan, A. Zaykov, Z. Havlas, J. Michl, and N. Marom “Inverse Design of Tetracene Polymorphs with Enhanced Singlet Fission Performance by Property-Based Genetic Algorithm Optimization”, *Chem. Mater.*, **35**, 1373 (2023)
- 69) X. Wang, S. Gao, A. Wang, B. Wang, Y. Guo, and N. Marom “Multiple resonance induced thermally activated delayed fluorescence: Effect of chemical modification” *Electronic Structure* **5**, 014010 (2023). (invited paper, “Focus on Excited States of Condensed Matter”)
- 70) M. J. A. Jardine, D. Dardzinski, M. Yu, A. Purkayastha, A.-H. Chen, Y.-H. Chang, A. Engel, V. N. Strocov, M. Hocevar, C. J. Palmstrøm, S. M. Frolov, and N. Marom, “First Principles Assessment of CdTe as a Tunnel Barrier at the α -Sn/InSb Interface”, *ACS Applied Materials & Interfaces* **15**, 16288 (2023)
- 71) S. Moayedpour, I. Bier, W. Wen, D. Dardzinski, O. Isayev, and N. Marom “Structure Prediction of Epitaxial Organic Interfaces with OGRE, demonstrated for TCNQ on TTF”, *J. Phys. Chem. C*, **127**, 10398 (2023) (invited paper, “Early-Career and Emerging Researchers in Physical Chemistry Volume 2” Special Issue)
- 72) R. Batabyal, S. Zelzer, A. P. Romagosa, D. Dardzinski, F. Corsetti, N. Marom, P. Krogstrup “Origin of Surface and Subband States at the InAs(111)A Surface”, *Phys. Rev. Materials*, **7**, 066201 (2023)
- 73) D. O’Connor, I. Bier, R. Tom, A. M. Hiszpanski, B. A. Steele, and N. Marom “Ab-Initio Crystal Structure Prediction of the Energetic Materials LLM-105, RDX, and HMX”, *Crystal Growth & Design* **23**, 6275 (2023)
- 74) X. Wang, A. Wang, M. Zhao, N. Marom “Inverted Lowest Singlet and Triplet Excitation Energy Ordering of Graphitic Carbon Nitride Flakes” *J. Phys. Chem. Lett.* **14**, 10910 (2023)
- 75) X. Wang, S. Gao, Y. Luo, X. Liu, R. Tom, K. Zhao, V. Chang, N. Marom “Computational Discovery of Intermolecular Singlet Fission Materials Using Many-Body Perturbation Theory” *J. Phys. Chem. C* **128**, 7841 (2024) (invited review)
- 76) P. B. Klar, D. G. Waterman, T. Gruene, D. Mullick, Y. Song, J. B. Gilchrist, C. D. Owen, W. Wen, I. Biran, L. Houben, N. Regev-Rudzki, R. Dzikowski, N. Marom, L. Palatinus, P. Zhang, L. Leiserowitz, M. Elbaum “Cryo-tomography and 3D Electron Diffraction Reveal the Polar Habit and Chiral Structure of the Malaria Pigment Crystal Hemozoin” *ACS Cent. Sci.* **10**, 1504 (2024)
- 77) N. Krainova, H. M. Johnson, R. Lampande, S. Gao, N. Marom, B. P. Rand, N. C. Giebink “Vacuum deposition of $\chi^{(2)}$ nonlinear organic single crystal films on silicon” *Appl. Phys. Lett.* **125**, 031104 (2024)
- 78) L. M. Hunnisett et al. “The seventh blind test of crystal structure prediction: Structure generation methods” *Acta Cryst. B* **80**, 517 (2024)

- 79) L. M. Hunnisett *et al.* “The seventh blind test of crystal structure prediction: Structure ranking methods” *Acta Cryst. B* **80**, 548 (2024)
- 80) M. J. A. Jardine, D. Dardzinski, Z. Cai, V. N. Strocov, M. Hocevar, C. J. Palmstrøm, S. M. Frolov, and N. Marom “First-Principles Assessment of ZnTe and CdSe as Prospective Tunnel Barriers at the InAs/Al Interface” *ACS Applied Materials & Interfaces* **17**, 5462 (2025)
- 81) S. Toso, D. Dardzinski, L. Manna, N. Marom “Structure Prediction of Ionic Epitaxial Interfaces with OGRE Demonstrated for Colloidal Heterostructures of Lead Halide Perovskites” *ACS Nano* **19**, 5326 (2025)
- 82) S. Gao, X. Liu, Y. Luo, X. Wang, K. Zhao, V. Chang, B. Schatschneider, N. Marom “PAH101: A GW+BSE Dataset of 101 Polycyclic Aromatic Hydrocarbon (PAH) Molecular Crystals” *Scientific Data* **12**, 679 (2025)
- 83) S. Gao, Y. Luo, X. Liu, N. Marom “Predicting the excited-state properties of crystalline organic semiconductors using GW+BSE and machine learning” *Digital Discovery* **4**, 1306 (2025) (highlighted in the themed collection “Celebrating International Women’s Day 2026: Women in Digital Discovery”)
- 84) S. Nishihaya, M. J. A. Jardine, H. S. Inbar, A. Goswami, J. T. Dong, A. N. Engel, Y.-H. Chang, C. P. Dempsey, M. Hashimoto, D. Lu, N. Marom, C. J. Palmstrøm “Near-half-metallic state in the half Heusler PtMnSb film on a III-V substrate” *Physical Review Materials* **9**, 044403 (2025)
- 85) K. Singh Nayal, D. O’Connor, R. Zubatyuk, D. M. Anstine, Y. Yang, R. Tom, W. Deng, K. Tang, N. Marom, and O. Isayev “Efficient Molecular Crystal Structure Prediction and Stability Assessment with AIMNet2 Neural Network Potentials” *Crystal Growth & Design* **25**, 9092 (2025)
- 86) Y. Yang, R. Tom, J. A. G. L. Wui, J. M. Moussa, and N. Marom “Genarris 3.0: Generating Close-Packed Molecular Crystal Structures with Rigid Press” *J. Chem. Theory Comput.* **21**, 11318 (2025)
- 87) V. Gharakhanyan, L. Barroso-Luque, Y. Yang, M. Shuaibi, K. Michel, D. S. Levine, M. Dzamba, X. Fu, M. Gao, X. Liu, H. Ni, K. Noori, B. M. Wood, M. Uyttendaele, A. Boromand, C. L. Zitnick, N. Marom, Z. W. Ulissi, A. Sriram “Open Molecular Crystals 2025 (OMC25) Dataset and Models” *Scientific Data*, **13**, 354 (2026)
- 88) H. Ni, K. Larkin, W. Wen, S. Moayedpour, R. Tom, I. Bier, D. Dardzinski, and N. Marom “Structure Prediction of Organic/Inorganic Interfaces with Genarris” *J. Chem. Theory Comput.*, **22**, 4835 (2026)
- 89) V. Gharakhanyan, Y. Yang, L. Barroso-Luque, M. Shuaibi, D. S. Levine, K. Michel, V. Bernat, M. Dzamba, X. Fu, M. Gao, X. Liu, K. Noori, L. J. Purvis, T. Rao, B. M. Wood, A. Rizvi, M. Uyttendaele, A. J. Ouderkerk, C. Daraio, C. L. Zitnick, A. Boromand, N. Marom, Z. W. Ulissi, A. Sriram “FastCSP: Accelerated Molecular Crystal Structure Prediction with Universal Model for Atoms” *arXiv* 2508.02641 (2025).
- 90) S. A. Ekahana, A. Tiwari, S. Sasmal, Z. Cai, R. K. Bandapelli, I. Kao, J. Tang, C. Min, T. Qian, K. Watanabe, T. Taniguchi, N. Ni, Q. Ma, C. Jozwiak, E. Rotenberg, A. Bostwick, S. Singh, N. Marom, J. Katoch “Visualization of Tunable Electronic Structure of Monolayer TaIrTe₄” *arXiv* 2601.11504 (2026), *Nature Communications*, in press
- 91) Z. Cai, M. J. A. Jardine, M. Yu, C. Min, J. Wu, H. Liu, D. Dardzinski, C. J. Palmstrøm, and N. Marom “Combining Quasiparticle Self-Consistent GW and Machine-Learned DFT+U to Assess Half-Metallicity in Co- and Ni-Based Heuslers” *arXiv* 2602.20621 (2026).
- 92) Y. Luo, X. Chen, S. Chen, K. Zhao, F. Simini, M. Del Ben, and N. Marom “OSC700: A GW+BSE Dataset of 700 Organic Semiconductor (OSC) Crystals with an LLM-Assisted Data Extraction Agent”, *ChemRxiv* DOI: 10.26434/chemrxiv.15005428/v1 (2026).
- 93) X. Chen, Y. Yang, J. Huang, X. Wu, and N. Marom “Structure Prediction of Multi-Component Molecular Crystals with Genarris 4.0” *ChemRxiv* DOI: 10.26434/chemrxiv.15005842/v1 (2026)
- 94) H. T. Kok, C. J. Su, P. Mastracco, H. Ni, M. Levy Greenberg, X. Zhou, S. V. Sundar, H. M. Johnson, M. Rzeszutko, P. Raghunathan, R. D. Priestley, Q. C. Burlingame, Y. L. Loo, N. C. Giebink, O. Yaffe, Y. H. Geerts, N. Marom, P. Clancy, B. P. Rand “Thin-Film Crystallization of Chiral Organics: Strain Accommodation of Scalemic BINAP in a Racemic Framework”, submitted

Invited Talks at Scientific Meetings:

- 1) N. Marom, J. Bernstein, J. Garel, A. Tkatchenko, E. Joselevich, L. Kronik, and O. Hod "Stacking and Registry Effects in Layered Materials: The Case of Hexagonal Boron Nitride", *XIX International Materials Research Congress (IMRC)*, Cancun, Mexico 08/'10.
- 2) N. Marom "Electronic Structure of Dye-Sensitized TiO₂ Clusters from G₀W₀", *Computational Surface Science - CompSurf 2011*, Santa Barbara, CA, USA 08/'11.
- 3) N. Marom "Electronic Structure of Dye-Sensitized TiO₂ Clusters from G₀W₀", *ES12: The 24th Annual Workshop on Recent Developments in Electronic Structure Theory*, Wake Forest University, NC, USA 06/'12.
- 4) N. Marom "Making Supercomputers Work", *Density Functional Theory and Beyond with Numeric Atom-Centered Orbitals*, Free University, Berlin, Germany 08/'12.
- 5) N. Marom "Electronic Structure of Dye-Sensitized TiO₂ Clusters from G₀W₀", *53rd Sanibel Symposium*, St. Simons Island, GA, USA 02/'13.
- 6) N. Marom "The Role of Many-Body Dispersion Interactions in Molecular Crystals", *2013 March Meeting of the American Physical Society*, Baltimore, MD, USA 03/'13.
- 7) N. Marom "Electronic Structure of Dye-Sensitized TiO₂ Clusters" *XXII International Materials Research Congress (IMRC)*, Cancun, Mexico 08/'13.
- 8) N. Marom "First Principles Modeling of Molecular Crystals" *Mini Symposium in Honor of Leslie Leiserowitz's 80th Birthday: A scientific Endeavor After Retirement*, Rehovoth, Israel, 04/'14.
- 9) N. Marom "Integrating Concepts- Cluster Structure Prediction and Spectroscopy" (invited tutorial) *Hands-on Summer School: Electronic Structure Theory for Materials and (Bio)molecules*, Los Angeles, CA, USA 07/'14.
- 10) N. Marom "Accurate Description of the Electronic Structure of Organic Semiconductors by GW Methods" *32nd International Conference on the Physics of Semiconductors (ICPS)*, Austin, TX, USA 08/'14.
- 11) N. Marom "First Principles Modeling of Molecular Crystals" *XXIII International Materials Research Congress (IMRC)*, Cancun, Mexico 08/'14.
- 12) N. Marom "Accurate Description of the Electronic Structure of Organic Semiconductors by GW Methods" *Addressing Challenges for First-Principles Based Modeling of Molecular Materials*, Lausanne, Switzerland, 08/'14.
- 13) N. Marom "Accurate Description of the Electronic Structure of Organic Semiconductors by GW Methods" *3rd workshop of the International Max Planck Research School (IMPRS) for Functional Interfaces in Physics and Chemistry*, Schloss Ringberg, Germany 02/'15.
- 14) N. Marom "Many-Body Dispersion Interactions in Molecular Crystals" *249th American Chemical Society (ACS) National Meeting & Exposition*, Denver, CO, USA 03/'15.
- 15) N. Marom "Accurate Description of the Electronic Structure of Organic Semiconductors by GW Methods" *The Louisiana Alliance for Simulation Guided Materials Applications (LA-SiGMA) Technical Conference*, Baton Rouge, LA, USA 04/'15.
- 16) N. Marom "Accurate Description of the Electronic Structure of Organic Semiconductors by GW Methods" *The 2015 Southeastern Theoretical Chemistry Association (SETCA) Annual Meeting*, Orlando, FL, USA 05/'15.
- 17) N. Marom "Toward Computational Design of Cluster-Based Functional Nano-Structures" *Theory of Metal Atoms, Clusters and Nanoparticles Stabilized by Organic Matter Workshop*, Helsinki, Finland 06/'15.
- 18) N. Marom "Toward Computational Design of Cluster-Based Functional Nano-Structures" *Recent Advances in Computational Modeling for Energy Applications*, Haifa, Israel 07/'15.
- 19) N. Marom "Accurate Description of the Electronic Structure of Organic Semiconductors by GW Methods" *Multiscale Simulations of Organic Electronic Materials*, Telluride, CO, USA 07/'15.
- 20) N. Marom "Introduction to DFT and its Applications to Defects in Semiconductors" (invited tutorial) *International Conference on Defects in Semiconductors (ICDS)*, Helsinki, Finland 07/'15.
- 21) N. Marom "Crystal Structure Prediction with GAtor" *Sixth Blind Test of Organic Crystal-Structure Prediction Methods*, Cambridge, UK 10/'15.

- 22) N. Marom "Toward Computational Design of Cluster-Based Functional Nano-Structures" *High Throughput Materials Discovery: Perspectives and Challenges in Theory and Experiment*, Tel-Aviv, Israel 02/'16.
- 23) N. Marom "Toward Computational Design of Cluster-Based Functional Nano-Structures" *56th Sanibel Symposium*, St. Simons Island, GA, USA 02/'16.
- 24) N. Marom "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *PPG Materials Innovations Symposium*, Pittsburgh, PA, USA 05/'16.
- 25) N. Marom "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *The 2016 Southeastern Theoretical Chemistry Association (SETCA) Annual Meeting*, Tallahassee, FL, USA 05/'16.
- 26) N. Marom "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *Charge and Energy Transfer in Photoreactions and Photodynamics*, Telluride, CO, USA 07/'16.
- 27) N. Marom "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *Electronic Structure Theory with Numeric Atom-Centered Basis Functions- FHI-aims Users' and Developers' Meeting*, Munich, Germany 07/'16.
- 28) N. Marom "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *Science 2016—Game Changers*, Pittsburgh, PA, USA 07/'16.
- 29) N. Marom "Accurate Description of the Electronic Structure of Organic Semiconductors by GW Methods" *EMN Meeting on Computation and Theory 2016*, Las Vegas, NV, USA 10/'16.
- 30) N. Marom "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *Understanding Many-Body Systems with Machine Learning III: Collective Variables in Quantum Mechanics*, Los Angeles, CA, USA 11/'16.
- 31) N. Marom "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *The 30th Annual Center for Simulation Physics (CSP) Workshop: Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, Athens, GA, USA 02/'17.
- 32) N. Marom "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *2017 March Meeting of the American Physical Society*, New Orleans, LA, USA 03/'17.
- 33) N. Marom "Opportunities for Machine Learning in Structure Prediction and Design of Molecular Crystals" *CMU Symposium on Machine Learning in Science and Engineering – 2017*, Pittsburgh, PA, USA 05/'17.
- 34) N. Marom "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *100th Canadian Chemistry Conference and Exhibition*, Toronto, ON, Canada 06/'17.
- 35) N. Marom "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *Interface Morphology Prediction with Robust and Efficient Structure Search (IMPRESS)*, Helsinki, Finland 06/'17.
- 36) N. Marom "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *2nd Israeli Conference on Computational Modeling of Molecules and Solids*, Tel-Aviv, Israel, 07/'17.
- 37) N. Marom "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *SPIE Optics+Photonics*, San Diego, CA, USA 08/'17.
- 38) N. Marom "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *254th ACS National Meeting & Exposition*, Washington, DC, USA 08/'17.
- 39) N. Marom "Crystal Structure Prediction with GAtor and Genarris" *Smoky Mountains Computational Sciences & Engineering Conference (SMC)*, Gatlinburg, TN, USA 08/'17.
- 40) N. Marom "The Complex High-Dimensional Energy Landscapes of Molecular Crystals" *Complex High-Dimensional Energy Landscapes Tutorials*, Los Angeles, CA, USA 09/'17.
- 41) N. Marom "Crystal Structure Prediction with GAtor and Genarris" *Workshop I: Optimization and Optimal Control for Complex Energy and Property Landscapes*, Los Angeles, CA, USA 10/'17.
- 42) N. Marom "Crystal Structure Prediction with GAtor and Genarris" *The 18th Israel Materials Engineering Conference (IMEC-18)*, Dead Sea, Israel, 02/'18.
- 43) N. Marom "Crystal Structure Prediction with GAtor and Genarris" *TMS 2018 Annual Meeting & Exhibition*, Phoenix, AZ, USA, 03/'18.
- 44) N. Marom "Molecular Crystal Structure Prediction with the GAtor Genetic Algorithm" *Practical Quantum Mechanics for Electronic Materials*, Austin, TX, USA, 06/'18.

- 45) N. Marom “Molecular Crystal Structure Prediction with GAtor and Genarris” *Machine Learning in Science and Engineering (MLSE)*, Pittsburgh, PA, USA, 06/’18.
- 46) N. Marom “Molecular Crystal Structure Prediction with GAtor and Genarris” *Modern Approaches to Coupling Scales in Materials Simulations*, Lenggries, Bavaria, Germany, 07/’18.
- 47) N. Marom “Molecular Crystal Structure Prediction with GAtor and Genarris”, **Plenary talk**, *Conference on Computational Physics 2018 (CCP2018)*, Davis, CA, USA, 08/’18.
- 48) N. Marom “Molecular Crystal Structure Prediction with GAtor and Genarris” *Artificial Intelligence in Materials Science (AIMS)*, Gaithersburg, MD, USA, 08/’18.
- 49) N. Marom “Molecular Crystal Structure Prediction with GAtor” *Frontiers in Molecular Dynamics: Machine Learning, Deep Learning and Coarse Graining*, Tel-Aviv, Israel, 10/’18.
- 50) N. Marom “Computational discovery of New Materials for Singlet Fission in the Solid State” *The Canadian Institute for Advanced Research (CIFAR) Bio-inspired Solar Energy program meeting*, Montreal, Canada, 10/’18.
- 51) N. Marom “Molecular Crystal Structure Prediction with the GAtor Genetic Algorithm” *2018 MRS Fall Meeting*, Boston, MA, USA, 11/’18.
- 52) N. Marom “Computational discovery of New Materials for Singlet Fission in the Solid State” *2019 March Meeting of the American Physical Society*, Boston, MA, USA, 03/’19.
- 53) N. Marom “Structure Prediction and Discovery of Molecular Crystals with Enhanced Electronic Properties”, *2019 Workshop on Recent Developments in Electronic Structure Theory*, The University of Illinois at Urbana-Champaign, Urbana-Champaign, IL, USA 05/’19.
- 54) N. Marom “Molecular Crystal Structure Prediction with the GAtor Genetic Algorithm” *Middle Atlantic Regional Meeting (MARM) of the American Chemical Society*, Baltimore, MD, USA, 06/’19.
- 55) N. Marom “Computational discovery of New Materials for Singlet Fission in the Solid State” *6th annual BerkeleyGW workshop*, Oakland, CA, 06/’19.
- 56) N. Marom “Machine Learning Descriptors for Singlet Fission” *Machine Learning in Science and Engineering (MLSE)*, Atlanta, GA, 06/’19.
- 57) N. Marom “Property-Based Genetic Algorithm Optimization of Molecular Crystals for High Carrier Mobility” *24th International Conference on the Chemistry of the Organic Solid State (ICCOSS XXIV)*, New York, NY, 06/’19.
- 58) N. Marom “First Principles Simulations of Hybrid Interfaces,” *SPIE Optics+Photonics*, San Diego, CA, USA 08/’19.
- 59) N. Marom “Molecular Crystal Structure Prediction with Genarris and GAtor” *MS&T19 Technical Meeting and Exhibition*, Portland, OR, USA, 10/’19.
- 60) N. Marom “Molecular Crystal Structure Prediction with Genarris and GAtor” *Rational Solid Form Design Summit (RSFD)*, Boston, MA, USA, 10/’19.
- 61) N. Marom “First Principles Simulations of Hybrid Interfaces,” *Theory and Computation for 2D Materials*, Los Angeles, CA, USA 01/’20.
- 62) N. Marom “Genarris 2.0, A Random Structure Generator for Molecular Crystals” *FHI-aims Developers’ and Users’ Meeting*, Berlin, Germany 06/’20 (virtual).
- 63) N. Marom “Structure Prediction and Discovery of Molecular Crystals with Enhanced Electronic Properties”, *Summer School Materials 4.0*, Dresden, Germany 08/’20 (virtual).
- 64) N. Marom “A Machine Learned Model for Molecular Solid Form Volume Prediction” *The Crystal Structure Prediction Consortium (CSPC) Meeting*, Cambridge, UK 11/’20 (virtual).
- 65) N. Marom “Accurate Materials Predictions with DFT and Machine Learning” *The 2021 Hybrid³ Theory Training Workshop*, Durham, NC 01/’21 (virtual).
- 66) N. Marom “Applications of Machine Learning in Materials Simulations” *The Institute for Mathematical and Statistical Innovation (IMSI) conference on Mathematical and Computational Materials Science*, Chicago, IL 02/’21 (virtual).
- 67) N. Marom “Molecular crystal structure and shape prediction with Genarris, GAtor, and OGRE”, *The 2021 ACS Spring Meeting*, 04/’21 (virtual).

- 68) N. Marom “Structure prediction and discovery of molecular crystals with enhanced electronic properties” *The 2021 ACS Spring Meeting*, 04/’21 (virtual).
- 69) N. Marom “First principles simulations of topological interfaces” *The 2021 ACS Spring Meeting*, 04/’21 (virtual).
- 70) N. Marom “Machine Learning the Hubbard U Parameter in DFT+U Using Bayesian Optimization” *Virtual Materials Design 2021*, 07/’21 (virtual).
- 71) N. Marom “Applications of Machine Learning in First Principles Materials Simulations” *2021 Joint Nanoscience and Neutron Scattering User Meeting*, Oak Ridge, TN, USA, 08/’21 (virtual).
- 72) N. Marom “Applications of Machine Learning in First Principles Materials Simulations” *MolSSI’s Two-Phase Materials Science Workshop: “Molecular Chemistry Meets Materials Science”*, Blacksburg, VA, USA, 03/’22 (virtual).
- 73) N. Marom “Many-Body Perturbation Theory Meets Machine Learning to Discover Singlet Fission Materials” *Midwest Theoretical Chemistry Conference (MWTCC)*, Columbus, OH, USA, 06/’22 (virtual).
- 74) N. Marom “Optimizing the Crystal Packing of Tetracene for Singlet Fission by a Property-Based Genetic Algorithm” *The 2022 ACS Fall Meeting*, 08/’22 (virtual).
- 75) N. Marom “Finding Predictive Models for Singlet Fission by Machine Learning” *The 2022 ACS Fall Meeting*, 08/’22 (virtual).
- 76) N. Marom “First Principles Simulations of Hybrid Inorganic Interfaces” *WeSST – Web Seminar Series on Tribology*, 10/’22 (virtual).
- 77) N. Marom “Finding Predictive Models for Singlet Fission by Machine Learning” *ACS Publications Summit: Advances in the Physical Chemistry of Energy Materials Research: Insights from Early Career and Emerging Investigators*, 12/’22 (virtual).
- 78) N. Marom “Finding Predictive Models for Singlet Fission by Machine Learning” *The 2022 MRS Fall Meeting*, Boston, MA, USA 12/’22 (virtual).
- 79) N. Marom “Structure Prediction and Discovery of Molecular Crystals with Enhanced Electronic Properties” *2024 March Meeting of the American Physical Society*, Minneapolis, MN, USA, 03/’24.
- 80) N. Marom “Finding Predictive Models for Singlet Fission by Machine Learning” *Machine Learning in Chemical and Materials Sciences (MLCM) 2024*, Los Alamos, NM, USA 05/’24 (virtual).
- 81) N. Marom “Computational Discovery of New Materials for Singlet Fission in the Solid State” *Crystal Engineering Gordon Research Conference*, Newry, ME, USA, 06/’24.
- 82) N. Marom “Computational Discovery of OLED Materials” *SPIE Optics+Photonics*, San Diego, CA, USA 08/’24.
- 83) N. Marom “Computational Discovery of New Materials for Singlet Fission in the Solid State” *The 7th Computational Molecular Science (CMS) Meeting*, University of Warwick, UK 09/’24.
- 84) N. Marom “First Principles Simulations of Hybrid Inorganic Interfaces” *The 70th American Vacuum Society conference (AVS70)*, Tampa, FL, USA 11/’24.
- 85) N. Marom “Computational Discovery of New Materials for Singlet Fission in the Solid State” *The 2025 ACS Spring Meeting*, San Diego, CA, USA 03/’25.
- 86) N. Marom “Crystal Structure Prediction of Energetic Materials” *TMS 2025 Annual Meeting & Exhibition*, Las Vegas, NV, USA, 03/’25.
- 87) N. Marom “Computational Discovery of New Materials for Singlet Fission in the Solid State” *Machine Learning in Chemical and Materials Sciences (MLCM) 2025*, Santa Fe, NM, USA 05/’25
- 88) N. Marom “Computational Discovery of New Materials for Singlet Fission in the Solid State” *Midwest Theoretical Chemistry Conference (MWTCC)*, Detroit, MI, USA 05/’25
- 89) N. Marom “Predicting the Structure of Molecular Crystals by Computer Simulations” *Molecular Education and Research Consortium in Undergraduate computational chemistry (MERCURY) Conference*, Pittsburgh, PA, USA 07/’25
- 90) N. Marom “Crystal Structure Prediction of Energetic Materials with Machine Learned Interatomic Potentials” *AI for Energetics Workshop* (virtual) 08/’25

- 91) N. Marom "Computational Discovery of New Materials for Singlet Fission in the Solid State" *Lennard-Jones Centre-CECAM Meeting 2025: From electrons to atoms to molecules and materials*, Cambridge, UK 09/'25
- 92) N. Marom "Computational Discovery of New Materials for Singlet Fission in the Solid State" *MS&T25*, Columbus, OH, USA 10/'25
- 93) N. Marom "Predicting the Structure and Properties of Epitaxial Inorganic Interfaces" *The 248th ECS Meeting*, Chicago, IL, USA 10/'25
- 94) N. Marom "Computational Discovery of New Materials for Singlet Fission in the Solid State" *The 2026 ACS Spring Meeting*, Atlanta, GA, USA 03/'26.
- 95) N. Marom "Molecular Crystal Structure Prediction with Machine-Learned Interatomic Potentials" *Canadian Societies for Chemistry and Chemical Engineering 2026 Conferences and Exhibition (x2026)*, Toronto, Canada 05/'26.
- 96) N. Marom "Structure Prediction of Molecular Interfaces" *FHI-aims Developers' and Users' Meeting 2026*, Hamburg, Germany 06/'26.
- 97) N. Marom "Predicting the Structure and Properties of Molecular Crystals with Machine Learning" *Foundations of Process/product Analytics and Machine learning (FOPAM) 2026*, Decatur, GA, USA 07/'26
- 98) N. Marom "Molecular Crystal Structure Prediction with Machine-Learned Interatomic Potentials" *Twenty-Seventh Congress and General Assembly of the International Union of Crystallography (IUCr2026)*, Calgary, Canada 08/'26.
- 99) N. Marom "Predicting the Excited-State Properties of Molecular Crystals with GW+BSE and Machine Learning" *7th Berkeley Excited States Conference (BESC2026)*, Berkeley, CA, USA 08/'26.

Contributed Presentations at Scientific Meetings:

- 1) N. Marom, D. Naveh, B. D. Schultz, C. Adelman, C. J. Palmström, P. A. Crowell, and L. Kronik, "Dependence of spin injection on interfacial bonding in Fe/GaAs junctions", *Safed Summer School on Density Functional Theory*, Safed, Israel, 09/'07.
- 2) N. Marom, D. Naveh, B. D. Schultz, C. Adelman, C. J. Palmström, P. A. Crowell, and L. Kronik, "Dependence of spin injection on interfacial bonding in Fe/GaAs junctions", *26th Israeli Vacuum Society Annual Conference and Technical Workshop*, Herzlia, Israel, 10/'07.
- 3) N. Marom and L. Kronik, "Density functional theory of transition metal phthalocyanines", *27th Israeli Vacuum Society Annual Conference and Technical Workshop*, Herzlia, Israel, 10/'08.
- 4) N. Marom and L. Kronik, "Density functional theory of transition metal phthalocyanines", *Annual Symposium of the Lise Meitner-Minerva Center*, Jerusalem, Israel, 11/'08.
- 5) N. Marom and L. Kronik, "Electronic structure of transition metal phthalocyanines: a comparative density functional theory study", *2009 March Meeting of the American Physical Society*, Pittsburgh, PA, USA, 03/'09.
- 6) N. Marom and L. Kronik, "Density functional theory of transition metal phthalocyanines", *2nd Workshop on Computations in Nanotechnology*, Haifa, Israel, 05/'09.
- 7) N. Marom, A. Tkatchenko, M. Scheffler, and L. Kronik, "A balanced description of dispersive interactions and electronic structure using density functional theory: the case of metal-phthalocyanine dimers", *Workshop on Ab Initio Molecular Simulations: Toward a First-Principles Understanding of Materials Properties and Functions*, Berlin, Germany, 06/'09.
- 8) N. Marom, T. Körzdörfer, S. Kümmel, and L. Kronik, "Density functional theory calculations of photoelectron spectra: the case of organic semiconductors", *Light Energy for a Brighter Future*, London, UK, 07/'09.
- 9) N. Marom, A. Tkatchenko, M. Scheffler, and L. Kronik, "A balanced description of dispersive interactions and electronic structure using density functional theory: the case of metal-phthalocyanine dimers", *The 14th Israel Materials Engineering Conference (IMEC-14)*, Tel-Aviv, Israel, 12/'09.
- 10) N. Marom, A. Tkatchenko, M. Scheffler, and L. Kronik, "A balanced description of dispersive interactions and electronic structure using density functional theory: the case of metal-phthalocyanine dimers", *The 75th Meeting of the Israel Chemical Society (ICS)*, Tel-Aviv, Israel, 01/'10.

- 11) N. Marom, A. Tkatchenko, M. Scheffler, and L. Kronik, "A balanced description of dispersive interactions and electronic structure using density functional theory: the case of metal-phthalocyanine dimers", *2010 March Meeting of the American Physical Society*, Portland, OR, USA, 03/'10.
- 12) N. Marom, J. Bernstein, J. Garel, A. Tkatchenko, E. Joselevich, L. Kronik, and O. Hod "Stacking and Registry Effects in Layered Materials: The Case of Hexagonal Boron Nitride", *ES10: The 22nd Annual Workshop on Electronic Structure Methods*, Austin, TX, USA, 06/'10.
- 13) N. Marom, A. Tkatchenko, S. Kapishnikov, T. Straasø, J. Als-Nielsen, L. Leiserowitz, and L. Kronik "Understanding β -Hematin Crystallization: The Role of van der Waals interactions", *Ψ_k Conference 2010*, Berlin, Germany, 09/'10.
- 14) N. Marom, J. Bernstein, J. Garel, A. Tkatchenko, E. Joselevich, L. Kronik, and O. Hod "Stacking and Registry Effects in Layered Materials: The Case of Hexagonal Boron Nitride", *XV International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods*, Trieste, Italy 01/'11.
- 15) N. Marom, A. Tkatchenko, S. Kapishnikov, T. Straasø, J. Als-Nielsen, L. Leiserowitz, and L. Kronik "Structure and Formation of Synthetic Hemozoin: Insights From First Principles Calculations", *2011 March Meeting of the American Physical Society*, Dallas, TX, USA, 03/'11.
- 16) N. Marom, J. Bernstein, J. Garel, A. Tkatchenko, E. Joselevich, L. Kronik, and O. Hod "Stacking and Registry Effects in Layered Materials: The Case of Hexagonal Boron Nitride", *Materials Design in Chemical Compound Space*, Los Angeles, CA, USA 05/'11.
- 17) N. Marom, X. Ren, J. R. Chelikowsky, and L. Kronik "Electronic Structure of Copper Phthalocyanine from G_0W_0 Calculations" *ES11: The 23rd Annual Workshop on Electronic Structure Methods*, Philadelphia, PA, USA, 06/'11.
- 18) N. Marom "Electronic Structure of Dye-Sensitized TiO_2 Clusters from G_0W_0 " *16th ETSF Workshop on Electronic Excitations*, Turin, Italy, 09/'11.
- 19) N. Marom, M. Kim, and J. R. Chelikowsky "Cluster Structure Selection Based on High Vertical Electron Affinity: The Case of TiO_2 Clusters" *Conference on Computational Physics (CCP) 2011*, Gatlinburg, TN, USA, 10/'11.
- 20) N. Marom, M. Kim, and J. R. Chelikowsky "Cluster Structure Selection Based on High Vertical Electron Affinity: The Case of TiO_2 Clusters" *2012 March Meeting of the American Physical Society*, Boston, MA, USA, 02/'12.
- 21) L. Leiserowitz, N. Marom, R. A. DiStasio Jr., V. Atalla, S. Levchenko, S. Kapishnikov, J. R. Chelikowsky, and A. Tkatchenko "The Role of Many-Body Dispersion Interactions in Molecular Crystal Polymorphism" *2012 March Meeting of the American Physical Society*, Boston, MA, USA, 02/'12.
- 22) N. Marom "A First Principles Treatment of Polymorphism in Molecular Crystals Using Dispersion-Corrected Density Functionals", *The Annual Meeting of the American Crystallographic Association (ACA)*, Boston, MA, USA, 7/'12.
- 23) N. Marom and A. Tkatchenko "The Role of Many-Body Dispersion Interactions in Molecular Crystal Polymorphism" *Towards First-Principles Description of van der Waals Interactions in Complex Materials*, Lausanne, Switzerland, 10/'12.
- 24) N. Marom and T. Körzdörfer "A Consistent Starting Point for G_0W_0 ", *Scientific Workflows for Scattering Science*, Pasadena, CA, USA, 1/'13.
- 25) E. Salomon, P. Amsalem, N. Marom, L. Kronik, N. Koch, and T. Angot "Electronic Structure of CoPc Adsorbed onto Ag(111): Evidence for Molecule-Substrate Interaction Mediated by Co 3d Orbitals", *2013 March Meeting of the American Physical Society*, Baltimore, MD, USA, 03/'13.
- 26) N. Marom, F. Caruso, X. Ren, O. Hofmann, T. Körzdörfer, J. R. Chelikowsky, A. Rubio, M. Scheffler, and P. Rinke "Benchmark of GW Methods for Azabenzenes: Is the GW Approximation good Enough?" *2013 March Meeting of the American Physical Society*, Baltimore, MD, USA, 03/'13.
- 27) N. Marom and T. Körzdörfer "A Consistent Starting Point for G_0W_0 ", *The 7th International Workshop on Electronic Structure and Processes at Molecular-Based Interfaces (ESPMI VII)*, Rehovoth, Israel, 4/'13.
- 28) N. Marom and T. Körzdörfer "A Consistent Starting Point for G_0W_0 ", *Green's Function Methods: The Next Generation*, Toulouse, France, 6/'13.
- 29) N. Marom and T. Körzdörfer "A Consistent Starting Point for G_0W_0 ", *Materials for a Sustainable Energy Future I: Solar Cells*, Los Angeles, CA, USA 9/'13.

- 30) N. Marom, T. Körzdörfer, X. Ren, A. Tkatchenko, and J. R. Chelikowsky, "Size Effects in Dye-Sensitized TiO₂ Clusters" *2014 March Meeting of the American Physical Society*, Denver, CO, USA, 03/'14.
- 31) N. Marom, "Accurate Description of the Electronic Structure of Organic Semiconductors by GW Methods" *European Materials Research Society (E-MRS) 2014 Spring Meeting*, Lille, France, 05/'14.
- 32) S. Bhattacharya, B. H. Sonin, C. J. Jumonville, L. M. Ghiringhelli, and N. Marom "Computational Design of Nanoclusters by Property-Based Genetic Algorithms: Tuning the Electronic Properties of (TiO₂)_n Clusters" *Machine Learning for Many-Particle Systems*, Los Angeles, CA, USA 02/'15.
- 33) S. Bhattacharya, L. M. Ghiringhelli, and N. Marom "Property-Based Cascade Genetic Algorithm for Tailored Searches of Metal-Oxide Nano-Structures" *2015 March Meeting of the American Physical Society*, San Antonio, TX, USA, 03/'15.
- 34) N. Marom, S. Bhattacharya, and L. M. Ghiringhelli "Structure Matters More Than Size: Tuning the Electronic Properties of (TiO₂)_n Clusters" *2015 March Meeting of the American Physical Society*, San Antonio, TX, USA, 03/'15.
- 35) N. Marom, S. Bhattacharya, and L. M. Ghiringhelli "Computational Design of Nanoclusters by Property-Based Genetic Algorithms: Tuning the Electronic Properties of (TiO₂)_n Clusters" *XXIV International Materials Research Congress (IMRC)*, Cancun, Mexico 08/'15.
- 36) N. Marom, J. Knight, X. Wang, L. Gallandi, O. Dolgounitcheva, X. Ren, J. V. Ortiz, P. Rinke, T. Körzdörfer "Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules: A Benchmark of GW Methods" *2016 March Meeting of the American Physical Society*, Baltimore, MD, USA, 03/'16.
- 37) F. Curtis, X. Li, T. Rose, A. Vazquez-Mayagoitia, S. Bhattacharya, L. M. Ghiringhelli, and N. Marom "Gator: A First Principles Genetic Algorithm for Molecular Crystal Structure Prediction" *2018 March Meeting of the American Physical Society*, Los Angeles, CA, USA, 03/'18.
- 38) N. Marom "On the Possibility of Singlet Fission in Crystalline Quaterylene" *2018 Materials Research Society (MRS) Spring Meeting & Exhibit*, Phoenix, AZ, USA, 04/'18.
- 39) F. Curtis, T. Rose, and N. Marom "Evolutionary Niching in the Gator Genetic Algorithm for Molecular Crystal Structure Prediction", *Faraday Discussion: Methods and Applications of Crystal Structure Prediction*, Cambridge, UK, 07/'18.
- 40) N. Marom "Molecular Crystal Structure Prediction with the Gator Genetic Algorithm" *2018 AIChE Annual Meeting*, Pittsburgh, PA, USA, 10/'18.
- 41) R. Tom, I. Bier, T. Rose, H. O'Brien, and N. Marom "Genarris 2.0: A Random Structure Generator for Molecular Crystals" *2019 AIChE Annual Meeting*, Orlando, FL, USA, 11/'19.
- 42) X. Wang, R. Tom, X. Liu, D. Congreve, N. Marom "Energetics perspective on why there are so few triplet-triplet annihilation emitters" *The 2021 ACS Spring Meeting*, 04/'21 (virtual).
- 43) S. Yang, N. Schröter, S. Schuwalow, M. Rajpalk, K. Ohtani, P. Krogstrup, G. W. Winkler, J. Gukelberger, D. Gresch, G. Aepli, V. N. Strocov, R. M. Lutchyn, N. Marom "Electronic Structure of InAs and InSb Surfaces: Density Functional Theory and Angle-Resolved Photoemission Spectroscopy" *2022 March Meeting of the American Physical Society*, Chicago, IL, USA, 03/'22 (virtual).
- 44) S. Moayedpour, I. Bier, W. Wen, D. Dardzinski, O. Isayev, and N. Marom "Structure Prediction of Epitaxial Organic Interfaces with Ogre, demonstrated for TCNQ on TTF" *2024 March Meeting of the American Physical Society*, Minneapolis, MN, USA, 03/'24
- 45) N. Marom, O. Isayev, B. P. Rand, N. C. Giebink "DMREF: Informed Design of Epitaxial Organic Electronics and Photonics" *MGI PI Meeting*, Washington, DC, USA 07/'24
- 46) N. Marom, D. Dardzinski, S. Toso, L. Manna "Structure Prediction of Ionic Epitaxial Interfaces with Ogre Demonstrated for Colloidal Heterostructures of Lead Halide Perovskites" *APS global Physics Summit*, Anaheim, CA, USA 03/'25
- 47) N. Marom, X. Wang, A. Wang, M. Zhao "Inverted Lowest Singlet and Triplet Excitation Energy Ordering of Graphitic Carbon Nitride Flakes" *APS global Physics Summit*, Anaheim, CA, USA 03/'25
- 48) N. Marom Crystal "Structure Prediction with Genarris and Machine-Learned Interatomic Potentials" *2025 AIChE Annual Meeting*, Boston, MA, USA 11/'25
- 49) N. Marom Crystal "Molecular Crystal Structure Prediction with Machine-Learned Interatomic Potentials" *APS global Physics Summit*, Denver, CO, USA 03/'26

- 50) N. Marom Crystal “Molecular Crystal Structure Prediction with Machine-Learned Interatomic Potentials” *The 2026 ACS Spring Meeting*, Atlanta, GA, USA 03/’26
- 51) N. Marom, O. Isayev, B. P. Rand, N. C. Giebink “DMREF: Informed Design of Epitaxial Organic Electronics and Photonics” *MGI PI Meeting*, Washington, DC, USA 08/’26

Seminars and Colloquia:

- 1) “Applications of van der Waals Corrected Density Functional Theory”, *The University of Texas at Austin*, Austin, TX, USA, 10/’10
- 2) “Cluster Structure Selection Based on High Vertical Electron Affinity: The Case of TiO₂ Clusters” *Fritz-Haber-Institut der Max-Planck-Gesellschaft*, Berlin, Germany, 11/’11
- 3) “Electronic Structure of Dye-Sensitized TiO₂ Clusters from G₀W₀”, *The University of Texas at Austin*, Austin, TX, USA, 11/’11
- 4) “A First Principles Treatment of Polymorphism in Molecular Crystals Using Dispersion-Corrected Density Functional Theory”, *New York University*, New York, NY, USA, 02/’12
- 5) “Electronic Structure of Dye-Sensitized TiO₂ Clusters from G₀W₀”, *Tel-Aviv University*, Tel-Aviv, Israel, 03/’12
- 6) “Electronic Structure of Dye-Sensitized TiO₂ Clusters from G₀W₀”, *Hebrew University*, Jerusalem, Israel, 04/’12
- 7) “Electronic Structure of Dye-Sensitized TiO₂ Clusters from G₀W₀”, *Weizmann Institute of Science*, Rehovoth, Israel, 04/’12
- 8) “Electronic Structure of Dye-Sensitized TiO₂ Clusters from Many-Body Perturbation Theory”, *Caltech*, Pasadena, CA, USA 05/’12
- 9) “Electronic Structure of Dye-Sensitized TiO₂ Clusters from G₀W₀”, *Technische Universität München*, Munich, Germany, 06/’12
- 10) “Electronic Structure of Dye-Sensitized TiO₂ Clusters from G₀W₀”, *University of Potsdam*, Potsdam, Germany, 09/’12
- 11) “Electronic Structure of Dye-Sensitized TiO₂ Clusters from G₀W₀”, *Pennsylvania State University*, State College, PA, USA 12/’12
- 12) “The Interface Problem: A Many-Body Perturbation Theory Perspective”, *Caltech*, Pasadena, CA, USA 01/’13
- 13) “Electronic Structure of Dye-Sensitized TiO₂ Clusters from Many-Body Perturbation Theory”, *University of Minnesota*, Minneapolis, MN, USA 02/’13
- 14) “The Interface Problem: A Many-Body Perturbation Theory Perspective”, *Argonne National Laboratory*, Lemont, IL, USA 03/’13
- 15) “Quantum Theory for Solar Cell Materials”, *Cornell University*, Ithaca, NY, USA 04/’13
- 16) “Quantum Theory for Solar Cell Materials”, *University of Maryland*, College Park, MD, USA 04/’13
- 17) “How Quantum Theory Can Help Cure Malaria”, *Tulane University*, New Orleans, LA, USA 04/’13
- 18) “Quantum Theory for Solar Cell Materials”, *Tulane University*, New Orleans, LA, USA 04/’13
- 19) “The Interface Problem: A Many-Body Perturbation Theory Perspective”, *The University of Texas at Austin*, Austin, TX, USA, 4/’13
- 20) “Quantum Theory for Solar Cell Materials”, *University of Pennsylvania*, Philadelphia, PA, USA 05/’13
- 21) “Quantum Theory for Solar Cell Materials”, *Drexel University*, Philadelphia, PA, USA 05/’13
- 22) “Quantum Theory for Solar Cell Materials”, *Aix-Marseille University*, Marseille, France 06/’13
- 23) “First Principles Modeling of Molecular Crystals”, *Southeastern Louisiana University*, Hammond, LA, USA 09/’13
- 24) “Electronic Structure of Dye-Sensitized TiO₂ Clusters”, *Carnegie Mellon University*, Pittsburgh, PA, USA 09/’13
- 25) “First Principles Modeling of Molecular Crystals”, *University of Pittsburgh*, Pittsburgh, PA, USA 09/’13
- 26) “First Principles Modeling of Molecular Crystals”, *Tulane University*, New Orleans, LA, USA 09/’13
- 27) “First Principles Modeling of Molecular Crystals”, *Tel-Aviv University*, Tel-Aviv, Israel 10/’13

- 28) "Electronic Structure of Dye-Sensitized TiO₂ Clusters", *Bar-Ilan University*, Ramat-Gan, Israel 10/'13
- 29) "Electronic Structure of Dye-Sensitized TiO₂ Clusters", *Technion- Israel Institute of Technology*, Haifa, Israel 10/'13
- 30) "Electronic Structure of Dye-Sensitized TiO₂ Clusters", *Humboldt University*, Berlin, Germany 11/'13
- 31) "First Principles Modeling of Molecular Crystals", *Potsdam University*, Potsdam, Germany 11/'13
- 32) "The Interface Problem: A Many-Body Perturbation Theory Perspective", *Fritz-Haber-Institut der Max-Planck-Gesellschaft*, Berlin, Germany, 11/'13
- 33) "Electronic Structure of Dye-Sensitized TiO₂ Clusters", *Louisiana State University*, Baton Rouge, LA, USA 12/'13
- 34) "Electronic Structure of Dye-Sensitized TiO₂ Clusters", *Georgia Tech*, Atlanta, GA, USA 12/'13
- 35) "Electronic Structure of Dye-Sensitized TiO₂ Clusters", *Duke University*, Durham, NC, USA 01/'14
- 36) "First Principles Modeling of Molecular Crystals", *University of New Orleans*, New Orleans, LA, USA 01/'14
- 37) "First Principles Modeling of Molecular Crystals", *Louisiana State University*, Baton Rouge, LA, USA 02/'14
- 38) "Electronic Structure of Dye-Sensitized TiO₂ Clusters", *University of Louisiana at Lafayette*, Lafayette, LA, USA 04/'14
- 39) "Electronic Structure of Dye-Sensitized TiO₂ Clusters", *Louisiana Tech*, Ruston, LA, USA 05/'14
- 40) "Electronic Structure of Dye-Sensitized TiO₂ Clusters", *CNRS*, Grenoble, France 05/'14
- 41) "Electronic Structure of Dye-Sensitized TiO₂ Clusters", *Key Laboratory of Quantum Information, University of Science and Technology of China*, Hefei, China 06/'14
- 42) "Electronic Structure of Dye-Sensitized TiO₂ Clusters", *Department of Physics, University of Science and Technology of China*, Hefei, China 06/'14
- 43) "Electronic Structure of Dye-Sensitized TiO₂ Clusters", *Fudan University*, Shanghai, China 06/'14
- 44) "Structure Matters More than Size: Tuning the Electronic Properties of TiO₂ Clusters" *Tulane University*, New Orleans, LA, USA 09/'14
- 45) "Accurate Description of the Electronic Structure of Organic Semiconductors by GW Methods" *Technion-Israel Institute of Technology*, Haifa, Israel 11/'14
- 46) "Accurate Description of the Electronic Structure of Organic Semiconductors by GW Methods" *Technische Universität München*, Munich, Germany, 02/'15
- 47) "Toward Computational Design of Functional Nanostructures" *University of Central Florida*, Orlando, FL, 04/'15
- 48) "Accurate Description of the Electronic Structure of Organic Semiconductors by GW Methods" *Temple University*, Philadelphia, PA 05/'15
- 49) "Toward Computational Design of Functional Nanostructures" *Carnegie Mellon University*, Pittsburgh, PA, USA 10/'15
- 50) "Toward Computational Design of Functional Nanostructures" *University College London*, London, UK 10/'15
- 51) "Toward Computational Design of Functional Nanostructures" *Diamond Light Source*, Didcot, Oxfordshire, UK 10/'15
- 52) "Toward Computational Design of Functional Nanostructures" *University of Oxford*, Oxford, UK 10/'15
- 53) "Toward Computational Design of Functional Nanostructures" *Imperial College London*, London, UK 10/'15
- 54) "Toward Computational Design of Functional Nanostructures" *University of New Orleans*, New Orleans, LA, USA 11/'15
- 55) "Toward Computational Design of Functional Nanostructures" *Georgia Tech*, Atlanta, GA, USA 11/'15
- 56) "Toward Computational Design of Functional Nanostructures" *Auburn University*, Auburn, AL, USA 11/'15
- 57) "Toward Computational Design of Functional Nanostructures" *Loyola University New Orleans*, New Orleans, LA, USA 12/'15

- 58) "Toward Computational Design of Functional Nanostructures" *Stevens Institute of Technology*, Hoboken, NJ, USA 04/'16
- 59) "Toward Computational Design of Functional Nanostructures" *University of Pittsburgh*, Pittsburgh, PA, USA 05/'16
- 60) "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *Forschungszentrum Jülich*, Jülich, Germany 07/'16.
- 61) "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *Carnegie Mellon University*, Pittsburgh, PA, USA 12/'16
- 62) "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *Pennsylvania State University*, State College, PA, USA 01/'17
- 63) "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *University of Pittsburgh*, Pittsburgh, PA, USA 03/'17
- 64) "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *University of Illinois at Chicago*, Chicago, IL, USA 04/'17
- 65) "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *Argonne National Laboratory*, Lemont, IL, USA 04/'17
- 66) "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *Oak Ridge National Laboratory*, Oak Ridge, TN, USA 09/'17
- 67) "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *University of Kentucky*, Lexington, KY, USA 10/'17
- 68) "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *University of California Riverside*, Riverside, CA, USA 10/'17
- 69) "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *Wake Forest University*, Winston-Salem, NC, USA 12/'17
- 70) "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *University of Toronto*, Toronto, ON, Canada 01/'18
- 71) "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *University of North Carolina*, Chapel Hill, NC, USA 04/'18
- 72) "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *Duke University*, Durham, NC, USA 04/'18
- 73) "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *North Carolina State University*, Raleigh, NC, USA 04/'18
- 74) "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *SUNY Buffalo*, Buffalo, NY, USA 05/'18
- 75) "Effect of Crystal Packing on the Electronic Properties of Molecular Crystals" *U.S. Army Research Laboratory*, Aberdeen Proving Ground, MD, USA 10/'18
- 76) "Computational discovery of New Materials for Singlet Fission in the Solid State" *Technical University Munich*, Munich, Germany 12/'18
- 77) "Structure prediction of molecular crystals from first principles" Computational Chemistry and Materials Science Summer Institute (CCMS), *Lawrence Livermore National Laboratory*, Livermore, CA, USA 07/'19.
- 78) "Computational discovery of New Materials for Singlet Fission in the Solid State" Computational Chemistry and Materials Science Summer Institute (CCMS), *Lawrence Livermore National Laboratory*, Livermore, CA, USA 07/'19.
- 79) "Structure Prediction and Discovery of Molecular Crystals with Enhanced Electronic Properties", *IBM Research- Almaden*, Almaden, CA, USA 07/'19.
- 80) "Structure Prediction and Discovery of Molecular Crystals with Enhanced Electronic Properties", *University of Vermont*, Burlington, VT, USA 09/'19.
- 81) "Structure Prediction and Discovery of Molecular Crystals with Enhanced Electronic Properties", *Oregon State University*, Corvallis, OR, USA 10/'19.

- 82) "Structure Prediction and Discovery of Molecular Crystals with Enhanced Electronic Properties", [University of California Santa Barbara](#), Santa Barbara, CA, USA 11/'19.
- 83) "Structure Prediction and Discovery of Molecular Crystals with Enhanced Electronic Properties", [University of Colorado Boulder](#), Boulder, CO, USA 02/'20.
- 84) "Structure Prediction and Discovery of Molecular Crystals with Enhanced Electronic Properties", [National Renewable Energy Laboratory \(NREL\)](#), Golden, CO, USA 02/'20.
- 85) "Structure Prediction and Discovery of Molecular Crystals with Enhanced Electronic Properties", [Trinity College Dublin](#), Dublin, Ireland 06/'20 (virtual).
- 86) "Applications of Machine Learning in Materials Simulations", [Kansas State University](#), Manhattan, KS, USA 05/'21 (virtual).
- 87) "Applications of Machine Learning in Materials Simulations", [North Carolina State University](#), Raleigh, NC, USA 09/'21 (virtual).
- 88) "First Principles Simulations of Hybrid Inorganic Interfaces" [Rutgers University](#), Piscataway, NJ, USA 10/'21 (virtual).
- 89) "First Principles Simulations of Hybrid Inorganic Interfaces" [Caltech](#), Pasadena, CA, USA 10/'21 (virtual).
- 90) "Applications of Machine Learning in Materials Simulations", [George Washington University](#), Washington, DC, USA 04/'22 (virtual).
- 91) "Applications of Machine Learning in Materials Simulations" [GA-Tech](#), Atlanta, GA, USA 04/'22 (virtual).
- 92) "Applications of Machine Learning in Materials Simulations" [UT El Paso](#), El Paso, TX, USA 02/'23 (virtual).
- 93) "Structure Prediction of Molecular Crystals and Epitaxial Organic Interfaces" [Meta](#), Menlo Park, CA, USA 05/'23 (virtual).
- 94) "Structure Prediction and Property Optimization of Molecular Crystals with Genarris and Gator" [Meta](#), Menlo Park, CA, USA 02/'24 (virtual).
- 95) "First Principles Simulations of Hybrid Inorganic Interfaces" [Carnegie Mellon University](#), Pittsburgh, PA, USA 04/'24.
- 96) "Computational Discovery of New Materials for Singlet Fission in the Solid State" [UC San Diego](#), San Diego, CA, USA 05/'24.
- 97) "Predicting the Structure and Properties of Molecular Crystals with Machine Learning" [Los Alamos National Laboratory](#), Los Alamos, NM, USA 08/'25
- 98) "Predicting the Structure and Properties of Inorganic Epitaxial Interfaces", [University of Illinois Urbana-Champaign](#), Urbana, IL, USA 12/'25.

Presentations by Group Members:

- 1) [F. S. Curtis](#), A. Tkatchenko, and N. Marom "Many-Body Dispersion Interactions in Layered Materials and Molecular Crystals", [Hands-on Summer School: Electronic Structure Theory for Materials and \(Bio\)molecules](#), Los Angeles, CA, USA 07/'14.
- 2) [F. S. Curtis](#), A. Tkatchenko, and N. Marom "Many-Body Dispersion Interactions in Layered Materials and Molecular Crystals", [Physics and Engineering Physics Summer Research Colloquium](#), New Orleans, LA, USA 08/'14.
- 3) [J. Knight](#), X. Ren, P. Rinke, N. Marom "A Benchmark of GW Methods for electron Acceptors", [Physics and Engineering Physics Summer Research Colloquium](#), New Orleans, LA, USA 08/'14.
- 4) [B. H. Sonin](#), A. Vazquez-Mayagoitia, N. Romero, V. Blum, N. Marom "Profiling and Multi-Threading FHI-aims on the Blue Gene/Q" [Physics and Engineering Physics Summer Research Colloquium](#), New Orleans, LA, USA 08/'14.
- 5) [F. S. Curtis](#), A. Tkatchenko, and N. Marom "The Role of Dispersion Interactions in the Racemic and Enantiomeric forms of Alanine", [Machine Learning for Many-Particle Systems](#), Los Angeles, CA, USA 02/'15.
- 6) [F. S. Curtis](#), A. Tkatchenko, and N. Marom "The Role of Dispersion Interactions in the Racemic and Enantiomeric forms of Alanine", [SCALA 2015: Scientific Computing Around Louisiana](#), New Orleans, LA, USA 03/'15.

- 7) [S. Lohani](#), C. D. Maggio, and N. Marom “FHI-aims Benchmark on Cypress and Sphynx” *SCALA 2015: Scientific Computing Around Louisiana*, New Orleans, LA, USA 03/’15.
- 8) [J. Knight](#), X. Wang, L. Gallandi, X. Ren, P. Rinke, T. Körzdörfer, and N. Marom “Benchmark of GW Methods for Electron Acceptors” *SCALA 2015: Scientific Computing Around Louisiana*, New Orleans, LA, USA 03/’15.
- 9) [X. Wang](#), M. Zhao, and N. Marom “Formation and Annealing Behaviors of Qubit Centers in 4H-SiC from First-Principles” *SCALA 2015: Scientific Computing Around Louisiana*, New Orleans, LA, USA 03/’15.
- 10) [F. S. Curtis](#), A. Tkatchenko, and N. Marom "The Role of Dispersion Interactions in the Racemic and Enantiomeric forms of Alanine" *The 27th Annual Workshop on Recent Developments in Electronic Structure Theory (ES15)*, Seattle, WA, USA 06/’15.
- 11) [S. Lohani](#), C. D. Maggio, and N. Marom “FHI-aims Benchmark on Cypress and Sphynx” *The 27th Annual Workshop on Recent Developments in Electronic Structure Theory (ES15)*, Seattle, WA, USA 06/’15.
- 12) [X. Wang](#), J. Knight, L. Gallandi, O. Dolgounitcheva, J. V. Ortiz, X. Ren, P. Rinke, T. Körzdörfer, and N. Marom “Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules: A Benchmark of GW Methods” *The 27th Annual Workshop on Recent Developments in Electronic Structure Theory (ES15)*, Seattle, WA, USA 06/’15.
- 13) [S. Lohani](#), C. D. Maggio, and N. Marom “FHI-aims Benchmark on Cypress and Sphynx” *Hands-On Workshop Density-Functional Theory and Beyond: First-Principles Simulations of Molecules and Materials*, Berlin, Germany 07/’15.
- 14) [X. Wang](#), J. Knight, L. Gallandi, O. Dolgounitcheva, J. V. Ortiz, X. Ren, P. Rinke, T. Körzdörfer, and N. Marom “Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules: A Benchmark of GW Methods” *Hands-On Workshop Density-Functional Theory and Beyond: First-Principles Simulations of Molecules and Materials*, Berlin, Germany 07/’15.
- 15) [A. Polanco-Valdez](#), N. Rahman, and N. Marom “A Lattice-Matching Algorithm for Layered Heterostructures” *The Louisiana Alliance for Simulation Guided Materials Applications (LA-SiGMA) Symposium*, Baton Rouge, LA, USA 07/’15 [2nd place in the LA-SiGMA REU poster competition].
- 16) [X. Wang](#), J. Knight, L. Gallandi, O. Dolgounitcheva, J. V. Ortiz, X. Ren, P. Rinke, T. Körzdörfer, and N. Marom “Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules: A Benchmark of GW Methods” *Physics and Engineering Physics Summer Research Colloquium*, New Orleans, LA, USA 08/’15.
- 17) [A. Polanco-Valdez](#), [N. Rahman](#), and N. Marom “A Lattice-Matching Algorithm for Layered Heterostructures” *Physics and Engineering Physics Summer Research Colloquium*, New Orleans, LA, USA 08/’15.
- 18) [S. Lohani](#), C. D. Maggio, and N. Marom “FHI-aims Benchmark on Cypress and Sphynx” *Physics and Engineering Physics Summer Research Colloquium*, New Orleans, LA, USA 08/’15.
- 19) [X. Wang](#), J. Knight, L. Gallandi, O. Dolgounitcheva, J. V. Ortiz, X. Ren, P. Rinke, T. Körzdörfer, and N. Marom “Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules: A Benchmark of GW Methods” *23rd Conference on Current Trends in Computational Chemistry*, Jackson, MS, USA 11/’15.
- 20) [X. Wang](#), J. Knight, L. Gallandi, O. Dolgounitcheva, J. V. Ortiz, X. Ren, P. Rinke, T. Körzdörfer, and N. Marom “Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules: A Benchmark of GW Methods” *56th Sanibel Symposium*, St. Simons Island, GA, USA 02/’16.
- 21) [X. Wang](#), T. Garcia, S. Monaco, B. Schatschneider, and N. Marom “Effect of Crystal Packing on the Excitonic Properties of Rubrene Polymorphs” *2016 March Meeting of the American Physical Society*, Baltimore, MD, USA, 03/’16.
- 22) [X. Wang](#), T. Garcia, S. Monaco, B. Schatschneider, and N. Marom “Effect of Crystal Packing on the Excitonic Properties of Rubrene Polymorphs” *2016 Simulators Meeting*, Pittsburgh, PA, USA, 05/’16.
- 23) [F. Curtis](#), X. Wang, and N. Marom “Effect of Packing Motifs on the Energy Ranking and Electronic Properties of Putative Crystal Structures of Tricyano-1,4-dithiino[c]-isothiazole” *2016 Simulators Meeting*, Pittsburgh, PA, USA, 05/’16.
- 24) [X. Li](#), F. Curtis, C. Schober, H. Oberhofer, and N. Marom “Genarris: Parallelized Configuration Space Screening of Molecular Crystals Aided by Harris Approximation” *Electronic Structure Theory with Numeric Atom-Centered Basis Functions- FHI-aims Users' and Developers' Meeting*, Munich, Germany 07/’16.
- 25) [F. Curtis](#), X. Li, and N. Marom “Molecular Crystal Structure Prediction with the GAtor Genetic Algorithm Package” *Understanding Many-Particle Systems with Machine Learning*, Los Angeles, CA, USA 10/’16 (Invited).
- 26) [X. Wang](#) “Effect of Crystal Packing on the Excitonic Properties of Rubrene Polymorphs” *The Behrend Computational Materials Meeting Focus on Atomic Level Methods and Applications*, Erie, PA, USA 11/’16 (Invited).
- 27) [F. Curtis](#), X. Wang, and N. Marom “Effect of Packing Motifs on the Energy Ranking and Electronic Properties of Putative Crystal Structures of Tricyano-1,4-dithiino[c]-isothiazole” *Understanding Many-Body Systems with Machine Learning III: Collective Variables in Quantum Mechanics*, Los Angeles, CA, USA 11/’16.

- 28) X. Wang "Case Study: BerkeleyGW Calculations on Molecular Crystals" *The BerkeleyGW Workshop*, Berkeley, CA, USA 01/'17 (invited).
- 29) X. Wang, T. Garcia, S. Monaco, B. Schatschneider, and N. Marom "Effect of Crystal Packing on the Excitonic Properties of Rubrene Polymorphs" *57th Sanibel Symposium*, St. Simons Island, GA, USA 02/'17.
- 30) X. Wang, S. Sanders, L. Campos, M. Sfeir, and N. Marom "Effect of co-crystallization on singlet fission efficiency in pentacene derivatives" *2017 March Meeting of the American Physical Society*, New Orleans, LA, USA, 03/'17.
- 31) F. Curtis, X. Wang, and N. Marom "Effect of Packing Motifs on the Energy Ranking and Electronic Properties of Putative Crystal Structures of Tricyano-1,4-dithiino[c]-isothiazole" *2017 March Meeting of the American Physical Society*, New Orleans, LA, USA, 03/'17.
- 32) X. Li, F. Curtis, C. Schober, A. Vazquez-Mayagoitia, H. Oberhofer, and N. Marom "Genarris: Parallelized Configuration Space Screening of Molecular Crystals Aided by Harris Approximation" *2017 March Meeting of the American Physical Society*, New Orleans, LA, USA, 03/'17.
- 33) F. Curtis, X. Li, and N. Marom "Evolutionary Niching: Cluster-Based Fitness in the Gator Genetic Algorithm" *CMU Symposium on Machine Learning in Science and Engineering – 2017*, Pittsburgh, PA, USA 05/'17.
- 34) X. Wang, S. Sanders, L. Campos, M. Sfeir, and N. Marom "Effect of co-crystallization on singlet fission efficiency in pentacene derivatives" *2017 Simulators Meeting*, Pittsburgh, PA, USA, 05/'17.
- 35) X. Liu, X. Wang, C. Cook, B. Schatschneider, and N. Marom "On the Possibility of Singlet Fission in Crystalline Quaterylene" *29th Annual Workshop on Recent Developments in Electronic Structure Methods (ES17)*, Princeton, NJ, USA 06/'17.
- 36) X. Wang, T. Garcia, S. Monaco, B. Schatschneider, and N. Marom "Effect of Crystal Packing on the Excitonic Properties of Rubrene Polymorphs" *29th Annual Workshop on Recent Developments in Electronic Structure Methods (ES17)*, Princeton, NJ, USA 06/'17.
- 37) T. Rose, F. Curtis, X. Li, and N. Marom "Evolutionary Niching: Cluster-Based Fitness in the Gator Genetic Algorithm" *Hands-on Workshop Density-Functional Theory and Beyond: Accuracy, Efficiency and Reproducibility in Computational Materials Science*, Berlin, Germany, 07/'17.
- 38) X. Wang, X. Liu, C. Cook, B. Schatschneider, and N. Marom "On the Possibility of Singlet Fission in Crystalline Quaterylene" *254th American Chemical Society National Meeting and Exposition*, Washington DC, USA 08/'17.
- 39) T. Rose, F. Curtis, X. Li, and N. Marom "Evolutionary Niching: Cluster-Based Fitness in the Gator Genetic Algorithm" *Workshop I: Optimization and Optimal Control for Complex Energy and Property Landscapes*, Los Angeles, CA, USA 10/'17.
- 40) T. Rose, F. Curtis, X. Li, and N. Marom "Evolutionary Niching: Cluster-Based Fitness in the Gator Genetic Algorithm" *Workshop III: Surrogate Models and Coarsening Techniques*, Los Angeles, CA, USA 11/'17.
- 41) X. Wang, X. Liu, C. Cook, B. Schatschneider, and N. Marom "On the Possibility of Singlet Fission in Crystalline Quaterylene" *The BerkeleyGW Workshop*, Berkeley, CA, USA 01/'18.
- 42) X. Wang, X. Liu, C. Cook, B. Schatschneider, and N. Marom "On the Possibility of Singlet Fission in Crystalline Quaterylene" *2018 March Meeting of the American Physical Society*, Los Angeles, CA, USA, 03/'18.
- 43) X. Liu, X. Wang, C. Cook, B. Schatschneider, and N. Marom "Phenyl-Substituted Acene Derivatives as Candidates for Intermolecular Singlet Fission" *2018 March Meeting of the American Physical Society*, Los Angeles, CA, USA, 03/'18.
- 44) X. Li, F. Curtis, T. Rose, C. Schober, A. Vazquez-Mayagoitia, K. Reuter, H. Oberhofer, and N. Marom "Genarris: Random Generation of Molecular Crystal Structures and Fast Screening with a Harris Approximation" *2018 March Meeting of the American Physical Society*, Los Angeles, CA, USA, 03/'18.
- 45) T. Rose, F. Curtis, and N. Marom "Evolutionary Niching in the Gator Genetic Algorithm for Molecular Crystal Structure Prediction" *2018 Simulator's Meeting*, Pittsburgh, PA, USA 05/'18
- 46) X. Liu, X. Wang, M. Yu, R. Tom and N. Marom "Accelerated Searching for Singlet Fission Materials- Feature Selection and Model Construction for GW+BSE Target Value with SISSO", *Machine Learning in Science and Engineering (MLSE)*, Pittsburgh, PA, USA 06/'18.
- 47) T. Rose, F. Curtis, and N. Marom "Evolutionary Niching in the Gator Genetic Algorithm for Molecular Crystal Structure Prediction" *Machine Learning in Science and Engineering (MLSE)*, Pittsburgh, PA, USA 06/'18
- 48) T. Rose, F. Curtis, and N. Marom "Evolutionary Niching in the Gator Genetic Algorithm for Molecular Crystal Structure Prediction" *Penn Conference in Theoretical Chemistry (PCTC)/ 30th Annual Workshop on Recent Developments in Electronic Structure Methods (ES18)*, Philadelphia, PA, USA 06/'18
- 49) X. Wang, X. Liu, C. Cook, B. Schatschneider, and N. Marom "Phenylated Acene Derivatives as Candidates for Intermolecular Singlet Fission" *Penn Conference in Theoretical Chemistry (PCTC)/ 30th Annual Workshop on Recent Developments in Electronic Structure Methods (ES18)*, Philadelphia, PA, USA 06/'18.
- 50) T. Rose, F. Curtis, and N. Marom "Evolutionary niching in the Gator genetic algorithm for molecular crystal structure prediction" *SciPy 2018*, Austin, TX, USA 07/'18.

- 51) I. Bier, N. Marom. "Engineering of high mobility molecular crystals using the Gator genetic algorithm" *FHI-aims Developers' and Users' Meeting 2018*, Technical University of Munich, Garching, Germany 07/'18.
- 52) X. Liu, X. Wang, M. Yu, R. Tom, and N. Marom "Accelerate Searching for Singlet Fission Materials — Feature Selection and Model Construction for GW+BSE Target Value with SISSO" *Artificial Intelligence for Materials Science (AIMS)*, Gaithersburg, MD, USA 08/'18.
- 53) I. Bier, N. Marom. "Engineering of high mobility molecular crystals using the Gator genetic algorithm" *Workshop on Artificial Intelligence for Materials Science (AIMS)*, NIST, Gaithersburg, MD, USA 08/'18.
- 54) X. Wang, M. Zhao, H. Bu, H. Zhang, X. He, A. Wang, and N. Marom "Formation and Annealing Behaviors of Qubit Centers in 4H-SiC from First-Principles" *Quantum Computing Materials Challenges*, Los Angeles, CA, USA 08/'18.
- 55) S. Yang, A. McGaughey, and N. Marom "Topological properties of SnSe by DFT calculations" *Quantum Computing Materials Challenges*, Los Angeles, CA, USA 08/'18.
- 56) X. Wang, M. Zhao, H. Bu, H. Zhang, X. He, A. Wang, and N. Marom "Formation and Annealing Behaviors of Qubit Centers in 4H-SiC from First-Principles" *PIRE:HYBRID 2018 Conference on materials for Quantum Computing*, Pittsburgh, PA, USA 10/'18.
- 57) S. Yang, A. McGaughey, and N. Marom "Topological properties of SnSe by DFT calculations" *PIRE:HYBRID 2018 Conference on materials for Quantum Computing*, Pittsburgh, PA, USA 10/'18.
- 58) X. Wang, X. Liu, R. Tom, C. Cook, B. Schatschneider, and N. Marom "Phenylated Acene Derivatives as Candidates for Intermolecular Singlet Fission" *2019 March Meeting of the American Physical Society*, Boston, MA, USA, 03/'19.
- 59) T. Rose, F. Curtis, and N. Marom "Evolutionary niching in the Gator genetic algorithm for molecular crystal structure prediction" *2019 March Meeting of the American Physical Society*, Boston, MA, USA, 03/'19.
- 60) M. Yu, X. Wang, X. Du, B. Schatschneider, H. Oberhofer, and N. Marom "Anomalous Pressure Dependence of the Electronic Properties of Molecular Crystals Explained by Changes in Intermolecular Electronic Coupling", *2019 March Meeting of the American Physical Society*, Boston, MA, USA, 03/'19.
- 61) A. Park, T. Rose, I. Bier, and N. Marom "Analysis of Genarris, structure generation package for molecular crystals", *Meeting of the Minds*, Pittsburgh, PA, USA, 05/'19.
- 62) M. Yu, X. Wang, X. Du, C. Kunkel, T. Garcia, S. Monaco, B. Schatschneider, H. Oberhofer, and N. Marom "Anomalous Pressure Dependence of the Electronic Properties of Molecular Crystals Explained by Changes in Intermolecular Electronic Coupling", *2019 Simulators Meeting*, Pittsburgh, PA, USA, 05/'19.
- 63) X. Wang, X. Liu, R. Tom, C. Cook, B. Schatschneider, and N. Marom "Phenylated Acene Derivatives as Candidates for Intermolecular Singlet Fission" *2019 Simulators Meeting*, Pittsburgh, PA, USA, 05/'19.
- 64) M. Yu, X. Wang, X. Du, C. Kunkel, T. Garcia, S. Monaco, B. Schatschneider, H. Oberhofer, and N. Marom "Anomalous Pressure Dependence of the Electronic Properties of Molecular Crystals Explained by Changes in Intermolecular Electronic Coupling", *2019 Workshop on Recent Developments in Electronic Structure Theory*, Urbana-Champaign, IL, USA 05/'19.
- 65) X. Wang, X. Liu, R. Tom, C. Cook, B. Schatschneider, and N. Marom "Phenylated Acene Derivatives as Candidates for Intermolecular Singlet Fission" *2019 Workshop on Recent Developments in Electronic Structure Theory*, Urbana-Champaign, IL, USA 05/'19.
- 66) S. Yang, C. Wu, and N. Marom "Topological Properties For SnSe/EuS and SnTe/CaTe Heterostructures" *2019 Workshop on Recent Developments in Electronic Structure Theory*, Urbana-Champaign, IL, USA 05/'19.
- 67) I. Bier, N. Marom. "Engineering of high mobility molecular crystals using the Gator genetic algorithm" *2019 Workshop on Recent Developments in Electronic Structure Theory*, Urbana-Champaign, IL, USA 05/'19.
- 68) R. Tom, I. Bier, T. Rose, H. O'Brien, and N. Marom "Genarris 2.0: Diverse Molecular Crystal Structure Generation by Space Groups" *2019 Workshop on Recent Developments in Electronic Structure Theory*, Urbana-Champaign, IL, USA 05/'19.
- 69) X. Wang, X. Liu, R. Tom, C. Cook, B. Schatschneider, N. Marom "Phenylated Acene Derivatives as Candidates for Intermolecular Singlet Fission", *Sixth Annual Workshop on BerkeleyGW*, Berkeley, CA, USA, 06/'19.
- 70) I. Bier, N. Marom. "Engineering of high mobility molecular crystals using the Gator genetic algorithm" *Machine Learning in Science and Engineering (MLSE)*, Atlanta, GA, 06/'19.
- 71) T. Rose, F. Curtis, and N. Marom "Evolutionary niching in the Gator genetic algorithm for molecular crystal structure prediction" *Machine Learning in Science and Engineering (MLSE)*, Atlanta, GA, 06/'19.
- 72) X. Wang, X. Liu, R. Tom, C. Cook, B. Schatschneider, N. Marom "Phenylated Acene Derivatives as Candidates for Intermolecular Singlet Fission", *2019 TDDFT School & Workshop: Excited states and dynamics*, Newark, NJ, USA, 08/'19.
- 73) M. Yu, X. Wang, X. Du, C. Kunkel, T. Garcia, S. Monaco, B. Schatschneider, H. Oberhofer, and N. Marom "Anomalous Pressure Dependence of the Electronic Properties of Molecular Crystals Explained by Changes in

Intermolecular Electronic Coupling”, *Penn Conference in Theoretical Chemistry (PCTC)*, Philadelphia, USA, 08/’19.

- 74) X. Wang, X. Liu, R. Tom, C. Cook, B. Schatschneider, and N. Marom “Phenylated Acene Derivatives as Candidates for Intermolecular Singlet Fission” *Penn Conference in Theoretical Chemistry (PCTC)*, Philadelphia, USA, 08/’19.
- 75) S. Yang, C. Wu, and N. Marom “Topological Properties For SnSe/EuS and SnTe/CaTe Heterostructures” *Penn Conference in Theoretical Chemistry (PCTC)*, Philadelphia, USA, 08/’19.
- 76) X. Wang, X. Liu, R. Tom, C. Cook, B. Schatschneider, and N. Marom “Phenylated Acene Derivatives as Candidates for Intermolecular Singlet Fission” *Hands-On DFT and Beyond: High-throughput screening and big-data analytics towards exascale computational materials science*, Barcelona, Spain, 08/’19.
- 77) R. Tom, I. Bier, T. Rose, H. O’Brien, and N. Marom “Genarris 2.0: Diverse Molecular Crystal Structure Generation by Space Groups” *Rational Solid Form Design Summit (RSFD)*, Boston, MA, USA, 10/’19.
- 78) I. Bier, R. Tom, and N. Marom “Genarris 2.0: Molecular crystal solid form volume estimation using Bayesian Inference” *Rational Solid Form Design Summit (RSFD)*, Boston, MA, USA, 10/’19.
- 79) S. Yang, C. Wu, and N. Marom “Topological Properties For SnSe/EuS and SnTe/CaTe Heterostructures” *Theory and Computation for 2D Materials*, Los Angeles, CA, USA 01/’20.
- 80) S. Yang, C. Wu, and N. Marom “Topological Properties For SnSe/EuS and SnTe/CaTe Heterostructures” *2021 March Meeting of the American Physical Society*, virtual, 03/’21.
- 81) M. Yu, S. Yang, C. Wu, and N. Marom “Machine learning the Hubbard U parameter in DFT+U using Bayesian optimization” *2021 March Meeting of the American Physical Society*, virtual, 03/’21.
- 82) S. Yang, I. Bier, W. Wen, J. Zhan, S. Moayedpour, N. Marom “Ogre: A Python Package for Molecular Crystal Surface Generation with Applications to Surface Energy and Crystal Habit Prediction” *2021 March Meeting of the American Physical Society*, virtual, 03/’21.
- 83) X. Wang, R. Tom, X. Liu, D. Congreve, N. Marom “An energetics perspective on why there are so few triplet-triplet annihilation emitters” *2021 March Meeting of the American Physical Society*, virtual, 03/’21.
- 84) X. Liu, R. Tom, S. Gao, N. Marom “Assessing Zethrene Derivatives as Singlet Fission Candidates Based on Multiple Descriptors” *2021 March Meeting of the American Physical Society*, virtual, 03/’21.
- 85) R. Tom, I. Bier, T. Rose, H. O’Brien, and N. Marom “Genarris 2.0: A Random Structure Generator for Molecular Crystals” *2021 March Meeting of the American Physical Society*, virtual, 03/’21.
- 86) I. Bier, N. Marom “Machine learned model for solid form volume estimation based on packing: Accessible surface and molecular topological fragments” *2021 March Meeting of the American Physical Society*, virtual, 03/’21.
- 87) X. Liu, R. Tom, X. Wang, C. Cook, B. Schatschneider, N. Marom “Pyrene-stabilized acenes as intermolecular singlet fission candidates: importance of exciton wave-function convergence” *2021 March Meeting of the American Physical Society*, virtual, 03/’21.
- 88) M. Yu, S. Yang, C. Wu, and N. Marom “Machine learning the Hubbard U parameter in DFT+U using Bayesian optimization” *2021 Spring Meeting of the American Chemical Society*, virtual, 04/’21.
- 89) X. Liu, R. Tom, X. Wang, C. Cook, B. Schatschneider, N. Marom “Pyrene-stabilized acenes as intermolecular singlet fission candidates: importance of exciton wave-function convergence” *2021 Spring Meeting of the American Chemical Society*, virtual, 04/’21.
- 90) I. Bier, N. Marom “Machine learned model for solid form volume estimation based on packing: Accessible surface and molecular topological fragments” *2021 Spring Meeting of the American Chemical Society*, virtual, 04/’21.
- 91) M. Yu, S. Moayedpour, S. Yang, D. Dardzinski, C. Wu, V. S. Pribiag, N. Marom “Dependence of the Electronic Structure of the EuS/InAs Interface on the Bonding Configuration”, *2022 March Meeting of the American Physical Society*, Chicago, IL, USA, 03/’22.
- 92) S. Moayedpour “Structure Prediction of Epitaxial Inorganic Interfaces by Lattice and Surface Matching with Ogre”, *2022 March Meeting of the American Physical Society*, Chicago, IL, USA, 03/’22.
- 93) S. Yang, D. Dardzinski, A. Hwang, D. I. Pikulin, G. W. Winkler, N. Marom “First Principles Feasibility Assessment of a Topological Insulator at the InAs/GaSb Interface”, *2022 March Meeting of the American Physical Society*, Chicago, IL, USA, 03/’22.
- 94) D. O’Connor “Crystal Structure Prediction of Energetic Materials and a Twisted Arene with Genarris and GAtor”, *2022 March Meeting of the American Physical Society*, Chicago, IL, USA, 03/’22.
- 95) R. Tom, S. Gao, N. Marom “Optimal polymorphs of tetracene for singlet fission”, *2022 March Meeting of the American Physical Society*, Chicago, IL, USA, 03/’22.
- 96) S. Gao, “Finding Predictive Descriptors for Singlet Fission by Machine Learning” *2022 March Meeting of the American Physical Society*, Chicago, IL, USA, 03/’22 (virtual).

- 97) B. Heischmidt, M. Yu, D. Dardzinski, J. Etheridge, S. Moayedpour, P. Crowell, N. Marom, V. Pribiag “Magnetic analysis of Heusler / III-V semiconductor interfaces using density functional theory” *2022 March Meeting of the American Physical Society*, Chicago, IL, USA, 03/’22.
- 98) M. J. Jardine, N. Marom, S. M. Frolov, A. Purkayastha, A. Chen, M. Hocevar, D. Dardzinski, M. Yu “Electronic structure of the InSb-CdTe- α Sn interface: using CdTe as a barrier” *2022 March Meeting of the American Physical Society*, Chicago, IL, USA, 03/’22.
- 99) D. O’Connor “Crystal Structure Prediction of Energetic Materials and a Twisted Arene with Genarris and Gator”, *2022 Simulators Meeting*, Pittsburgh, PA, USA, 05/’22.
- 100) S. Gao, “Finding Predictive Descriptors for Singlet Fission by Machine Learning” *2022 Simulators Meeting*, Pittsburgh, PA, USA, 05/’22.
- 101) M. J. Jardine, D. Dardzinski, M. Yu, N. Marom, A. Purkayastha, A.-H. Chen, M. Hocevar, Y. Hao, C. Palmstrøm, S. Frolov “Electronic structure of the InSb/CdTe/ α -Sn interface via DFT: using CdTe as a barrier” *2022 Workshop on Recent Developments in Electronic Structure Theory*, New-York, NY, USA, 05/’22.
- 102) W. Wen, S. Moayedpour, R. Tom, I. Bier, D. Dardzinski, N. Marom “Genarris 4.0: Random Structure Generator for Organic/Inorganic Interfaces” *2022 Workshop on Recent Developments in Electronic Structure Theory*, New-York, NY, USA, 05/’22.
- 103) S. Moayedpour, D. Dardzinski, S. Yang, A Hwang, and N. Marom “Structure prediction of epitaxial inorganic interfaces by lattice and surface matching with Ogre” *2022 Workshop on Recent Developments in Electronic Structure Theory*, New-York, NY, USA, 05/’22.
- 104) X. Liu, X. Wang, S. Gao, V. Chang, R. Tom, M. Yu, L. M. Ghiringhelli, and N. Marom “Finding Predictive Models for Singlet Fission by Machine Learning” *2022 Workshop on Recent Developments in Electronic Structure Theory*, New-York, NY, USA, 05/’22.
- 105) K. Grimes “Predicting Molecular Gaps with Minimal Data Using Active Learning”, *MS&T22*, Pittsburgh, PA, USA, 10/’22.
- 106) S. Gao, F. Simini, M. Del Ben, J. Deslippe, L. M. Ghiringhelli, X. Zhan, W. Huhn, B. Poczos, G. Fletcher, N. Marom “Background and Resources of MatML project” *MatSci ML Dungeon*, Portland, OR, USA 12/’22
- 107) S. Gao, X. Liu, K. Grimes, M. A. Abba, V. Chang, R. Tom, M. Yu, L. M. Ghiringhelli, D. O’Connor, F. Simini, K. K. Lee, B. Reich, N. Marom “Many-Body Perturbation Theory Meets Machine Learning to Discover Singlet Fission Materials” *C2SEMEP seminar*, Berkeley, CA, USA, 12/’22
- 108) M. J. A. Jardine, D. Dardzinski, M. Yu, A. Purkayastha, A.-H. Chen, Y.-H. Chang, A. Engel, V. N. Strocov, M. Hocevar, C. J. Palmstrøm, S. M. Frolov, and N. Marom, “First Principles Assessment of CdTe as a Tunnel Barrier at the α -Sn/Insb Interface”, *The 62nd Sanibel Symposium*, Augustine Beach, FL, USA 02/’23
- 109) S. Gao “Benchmarking time-dependent density functional theory for singlet excited states of thermally activated delayed fluorescence chromophores” *2023 March Meeting of the American Physical Society*, Las Vegas, NV, USA 03/’23
- 110) D. O’Connor, “Performance of Dispersion-Inclusive Density Functional Theory Methods for Energetic Materials” *2023 March Meeting of the American Physical Society*, Las Vegas, NV, USA 03/’23
- 111) D. Dardzinski, “First Principles Study of the Electronic Structure of the Ni₂MnIn/InAs and Ti₂MnIn/InSb Interfaces” *2023 March Meeting of the American Physical Society*, Las Vegas, NV, USA 03/’23
- 112) M. J. Jardine, S. Frolov, N. Marom, D. Dardzinski, M. Yu, A.-H. Chen, A. Engel, C. Palmstrøm, Y. Hao, M. Hocevar “Electronic structure of the InSb-CdTe- α Sn interface: using CdTe as a barrier” *2023 March Meeting of the American Physical Society*, Las Vegas, NV, USA 03/’23
- 113) X. Liu, X. Wang, S. Gao, V. Chang, R. Tom, M. Yu, L. M. Ghiringhelli, and N. Marom “Finding Predictive Models for Singlet Fission by Machine Learning” *Singlet Fission Workshop*, Denver, CO, USA, 06/’23.
- 114) R. Tom, S. Gao, Y. Yang, K. Zhao, I. Bier, E. A. Buchanan, A. Zaykov, Z. Havlas, J. Michl, and N. Marom “Inverse Design of Tetracene Polymorphs with Enhanced Singlet Fission Performance by Property-Based Genetic Algorithm Optimization” *Singlet Fission Workshop*, Denver, CO, USA, 06/’23.
- 115) D. O’Connor “Optimizing the Crystal Packing of Tetracene for Singlet Fission by a Property-Based Genetic Algorithm” *fpi15*, Raleigh, NC, USA 06/’23
- 116) D. O’Connor “Crystal Structure Prediction of Energetic Materials” *CECAM Workshop on Crystal Structure Prediction in Materials Discovery*, Liverpool, UK 07/’23
- 117) M. J. A. Jardine, A. Purkayastha, D. Dardzinski, M. Yu, N. Marom, A.-H. Chen, M. Hocevar, Y. Hao, A. Engel, C. Palmstrøm, S. Frolov “Electronic structure of the InSb/CdTe/ α -Sn interface via DFT: using CdTe as a barrier”, *Q-PHORIA Annual Conference 2023*, Pittsburgh, PA, 10/’23
- 118) M. J. A. Jardine, D. Dardzinski, C. J. Palmstrøm, M. Hocevar, S. M. Frolov, N. Marom “First principles assessment of prospective tunnel barriers at semiconductor/superconductor interfaces”, *Vienna Ab-initio Simulation Package (VASP) and Applications Conference*, Évora, Portugal, 02/’24

- 119) M. J. A. Jardine, D. Dardzinski, C. J. Palmstrøm, M. Hocevar, S. M. Frolov, N. Marom “First principles assessment of prospective tunnel barriers at semiconductor/superconductor interfaces”, *63rd Sanibel symposium*, St. Augustine Beach, FL, 02/’24
- 120) M. J. A. Jardine, D. Dardzinski, C. J. Palmstrøm, M. Hocevar, S. M. Frolov, N. Marom “First principles assessment of prospective tunnel barriers at semiconductor/superconductor interfaces”, *APS March Meeting*, Minneapolis, MN, 03/’24
- 121) R. Tom, S. Gao, Y. Yang, K. Zhao, I. Bier, E. A. Buchanan, A. Zaykov, Z. Havlas, J. Michl, and N. Marom “Inverse Design of Tetracene Polymorphs with Enhanced Singlet Fission Performance by Property-Based Genetic Algorithm Optimization” *APS March Meeting*, Minneapolis, MN, 03/’24
- 122) D. O'Connor, I. Bier, R. Tom, A. M. Hiszpanski, B. A. Steele, and N. Marom “Ab-Initio Crystal Structure Prediction of the Energetic Materials LLM-105, RDX, and HMX” *APS March Meeting*, Minneapolis, MN, 03/’24
- 123) Y. Yang, R. Tom, J. Moussa, N. Marom “Genarris 3.0: A random molecular crystal structure generator” *Crystal Engineering Gordon Research Conference*, Newry, ME, USA, 06/’24.
- 124) M. J. A. Jardine, D. Dardzinski, C. J. Palmstrøm, M. Hocevar, S. M. Frolov, N. Marom “First principles assessment of prospective tunnel barriers at semiconductor/superconductor interfaces” *The 7th Computational Molecular Science (CMS) Meeting*, University of Warwick, UK 09/’24
- 125) M. J. A. Jardine, “Using DFT to investigate prospective tunnel barriers at semiconductor/superconductor interfaces for MZM experiments” *West Virginia University*, Morgantown, WV, 12/’24
- 126) M. J. Jardine, D. Dardzinski, Z. Cai, V. N. Strocov, M. Hocevar, C. J. Palmstrom, S. M. Frolov, N. Marom, “First Principles Assessment of ZnTe and CdSe as Prospective Tunnel Barriers at the InAs/Al Interface” *NIST-JARVIS 4th Quantum Matters in Materials Science Workshop*, Rockville, MD, USA 02/’25
- 127) S. Toso, D. Dardzinski, H. Liu, L. Manna, N. Marom, “Structure Prediction of Ionic Epitaxial Interfaces with OGRE Demonstrated for Colloidal Heterostructures of Lead Halide Perovskites” *NIST-JARVIS 4th Quantum Matters in Materials Science Workshop*, Rockville, MD, USA 02/’25
- 128) N. Marom, Y. Luo, S. Gao, X. Liu, “Predicting the excited-state properties of crystalline organic semiconductors using GW+BSE and machine learning” *APS global Physics Summit*, Anaheim, CA, USA 03/’25
- 129) N. Marom, S. Gao, Y. Luo, X. Liu, R. Tom, K. Zhao, V. Chang, X. Wang, “Computational Discovery of Intermolecular Singlet Fission Materials Using Many-Body Perturbation Theory” *APS global Physics Summit*, Anaheim, CA, USA 03/’25
- 130) N. Marom, M. J. Jardine, D. Dardzinski, Z. Cai, V. N. Strocov, M. Hocevar, C. J. Palmstrom, S. Frolov “First Principles Assessment of ZnTe and CdSe as Prospective Tunnel Barriers at the InAs/Al Interface” *APS Global Physics Summit*, Anaheim, CA, USA 03/’25
- 131) N. Marom, M. J. Jardine, M. Yu, Z. Cai, J. Wu, D. Dardzinski, P. A. Crowell “Using Quasiparticle Self-Consistent GW and Density Functional Theory with Machine-Learned Hubbard U Corrections in Search of Half-Metallic Heuslers” *APS global Physics Summit*, Anaheim, CA, USA 03/’25
- 132) M. J. Jardine, D. Dardzinski, Z. Cai, V. N. Strocov, M. Hocevar, C. J. Palmstrom, S. M. Frolov, N. Marom, “First Principles Assessment of ZnTe and CdSe as Prospective Tunnel Barriers at the InAs/Al Interface” *Penn Conference on Theoretical Chemistry (PCTC) 2025*, Philadelphia, PA, USA 05/’25
- 133) Y. Luo, S. Gao, X. Liu, N. Marom, “Predicting the Excited-State Properties of Crystalline Organic Semiconductors Using GW+BSE and Machine Learning” *Penn Conference on Theoretical Chemistry (PCTC) 2025*, Philadelphia, PA, USA 05/’25
- 134) Y. Yang “Genarris 3.0: A Random Molecular Crystal Structure Generator with Rigid Press Geometry Optimization” *Machine Learning in Chemical and Materials Sciences (MLCM) 2025*, Santa Fe, NM, USA 05/’25
- 135) Y. Luo, S. Gao, X. Liu, N. Marom, “Predicting the Excited-State Properties of Crystalline Organic Semiconductors Using GW+BSE and Machine Learning” *Machine Learning in Chemical and Materials Sciences (MLCM) 2025*, Santa Fe, NM, USA 05/’25
- 136) M. J. Jardine, D. Dardzinski, Z. Cai, V. N. Strocov, M. Hocevar, C. J. Palmstrom, S. M. Frolov, N. Marom, “First Principles Assessment of ZnTe and CdSe as Prospective Tunnel Barriers at the InAs/Al Interface” *Electronic Structure Workshop 2025*, El Paso, TX, USA 06/’25
- 137) Y. Luo, S. Gao, X. Liu, N. Marom, “Predicting the Excited-State Properties of Crystalline Organic Semiconductors Using GW+BSE and Machine Learning” *Electronic Structure Workshop 2025*, El Paso, TX, USA 06/’25
- 138) Y. Yang, R. Tom, J. Moussa, N. Marom “Genarris 3.0: Generating Close-Packed Molecular Crystal Structures with Rigid Press” *APS global Physics Summit*, Denver, CO, USA 03/’26
- 139) H. Ni, K. Larkin, W. Wen, S. Moayedpour, R. Tom, I. Bier, D. Dardzinski, N. Marom “Structure Prediction of Organic/Inorganic Interfaces with Genarris” *APS global Physics Summit*, Denver, CO, USA 03/’26
- 140) Y. Yang, R. Tom, J. Moussa, N. Marom “Genarris 3.0: Generating Close-Packed Molecular Crystal Structures with Rigid Press” *2026 Penn Conference in Theoretical Chemistry (PCTC26)*, Philadelphia, PA, USA 05/’26

- 141) H. Ni, K. Larkin, W. Wen, S. Moayedpour, R. Tom, I. Bier, D. Dardzinski, N. Marom “Structure Prediction of Organic/Inorganic Interfaces with Genarris” *2026 Penn Conference in Theoretical Chemistry (PCTC26)*, Philadelphia, PA, USA 05/’26

Postgraduate Advising:

Malcolm Jardine (Fall 2023- Fall 2024)
Xiaopeng Wang (Fall 2014- Summer 2019; Tulane and CMU)
Farren S. Curtis (Spring 2018- Summer 2018)

Graduate Advising:

PhD:

Xiaochen Wang (Summer 2026- present)
Xinyu Wu (Fall 2025- present)
Zefeng Cai (Fall 2023- present)
Haoran Ni (Fall 2023- present)
Xuyan Chen (Fall 2023- present)
Jiayi Huang (Fall 2023- present)
Yi Yang (Spring 2023- present)
Yiqun Luo (Fall 2022- present)
Siyu Gao (Spring 2021- Summer 2025)
Derek Dardzinski (Summer 2020- Fall 2024)
Dana O’Connor (Fall 2019- Fall 2023)
Maituo Yu (Spring 2019- Spring 2023)
Wen Wen (Spring 2019- Summer 2022)
Saeed Moayedpour (Spring 2019- Summer 2022)
Rithwik Tom (Fall 2017- Summer 2022)
Xingyu (Alfred) Liu (Spring 2018- Spring 2022)
Imanuel (Manny) Bier (Fall 2017- Spring 2022)
Shuyang Yang (Fall 2017- Spring 2021)
Timothy Rose (Fall 2016- Summer 2020)
Farren S. Curtis (Spring 2014- Fall 2017; Tulane and CMU)

Co-advised PhD:

Brett Heischmidt (Summer 2020- Fall 2022, with Paul Crowell and Vlad Pribiag, U. Minnesota)
Malcolm Jardine (Fall 2020- Summer 2023, with Sergey Frolov, U. Pitt)

MS:

Yihao Yin (Fall 2026- present)
Jida Yang (Fall 2026- present)
Ziyue Sheng (Spring 2026- present)
Chenbo Min (Fall 2024- Spring 2026)
Hantian Liu (Spring 2024- Spring 2025)
Kevin Larkin (Fall 2022- Spring 2025)
Jiatian Wu (Fall 2021- Fall 2023)
Wenda Deng (Fall 2021- Spring 2023)
Kaiji Zhao (Fall 2021- Fall 2022)
Kehan Tang (Fall 2021- Fall 2022)
Yi Yang (Fall 2021- Fall 2022)
Jiashuo Wang (Fall 2021- Fall 2022)
Vincent Chang (Summer 2020- Spring 2022)
Shengjie Fu (Fall 2019- Fall 2020)
Siyu Gao (Fall 2019- Fall 2020)
Yun-Ting Hsieh (Fall 2019- Fall 2020)
Chunzhi Wu (Fall 2018- Fall 2019)
Maituo Yu (Fall 2017- Fall 2018)
Xingyu (Alfred) Liu (Fall 2016- Fall 2017)
Hongyi Liang (Fall 2016- Spring 2017)

Undergraduate Advising:

Carnegie Mellon University:

Siyu (Rain) Chen (Fall 2025- Spring 2026)
Christopher Berman (Spring 2023- Spring 2024)
Keya Sharma (Summer 2022- Spring 2024)
Brian Shin (Summer 2022- Summer 2023)
Keltin Grimes (Spring 2021- Spring 2023)
Ziyao Luo (Summer 2021- Spring 2022)
Seoyoung Joo (Summer 2021- Spring 2022)
Christian Frech (Spring 2021- Spring 2022)
Andrea Hwang (Fall 2018- Spring 2021)
Jiawei Zhan (University of Science and Technology of China, exchange student, Summer 2019)
Kylie Pearce (Cal-Poly Pomona, REU student, Summer 2019)
Anna Park (Summer 2018- Spring 2019)
Harriet O'Brien (Spring 2018- Summer 2019)
Xiong-Fei Du (Summer 2017- Fall 2017)
Max Farfel (Fall 2016- Summer 2017)

Tulane University:

Xiayue (Patrick) Li (Spring 2015- Summer 2016), *honors thesis: "Genarris: Parallelized Configuration Space Screening of Molecular Crystals Aided by Harris Approximation"*
Austin Polanco-Valdez, Stony Brook University (Summer 2015)
Katherine Cosburn, University of Toronto (Summer 2015)
Andrey Burin (Summer 2015)
Francesca Vaccaro, Loyola University New Orleans (Summer 2014- Summer 2015)
Joseph W. Knight (Summer 2014- Spring 2015), *honors thesis: "Benchmark of GW Methods for Electron Acceptors"*
Benjamin H. Sonin (Fall 2013- Spring 2014)
Christopher J. Jumonville (Fall 2013- Spring 2014)

Funding:

- Principal Investigator:
 - "CAREER: Structure Prediction and Design of Molecular Crystals with the Gator Genetic Algorithm", NSF, \$650,000, 08/01/16 – 12/31/21.
 - "Singlet Fission: Deriving Fundamental Insights from Computation", The Charles E. Kaufman Foundation, \$150,000, 09/01/17 – 08/31/19.
 - "W911NF-17-S-0002: Chemical Sciences: Structure Prediction and Design of Molecular Interfaces from First Principles", ARO, \$429,630, 07/01/18 – 09/30/22.
 - "Seed Project: Screening Polycyclic Aromatic Hydrocarbons for Singlet Fission Candidates", AFOSR, \$110,000, 06/01/18 – 05/31/19.
 - "Data Driven Discovery of Singlet Fission Materials", Scott Institute Seed Grant, \$75,303, 01/01/18-06/30/19.
 - "EAGER: MATDAT18 Type I: Collaborative Research: Data Driven Discovery of Singlet Fission Materials" (co-PI: Brian Reich, NCSU), NSF, \$237,841, 09/01/19- 8/31/20.
 - "Crystal Structure Prediction of Energetic Materials" DOE (sub-award through Lawrence Livermore National Laboratory), \$132,560, 02/07/20 – 9/30/20.
 - "Molecular Crystal Shape Prediction with Solvent Effects" DOE (sub-award through Lawrence Livermore National Laboratory), \$135,642, 11/01/20 – 9/30/21.
 - "Collaborative Research: Data Driven discovery of Singlet Fission Materials" (co-PI: Brian Reich, NCSU), NSF, \$400,000, 01/15/21- 01/14/24.
 - "Structure Prediction and Design of Molecular Crystals with Gator and Genarris" NSF, \$390,000, 01/01/22- 12/31/24

- “Collaborative Research: DMREF: Informed Design of Epitaxial Organic Electronics and Photonics” (Co-PIs Olexandr Isayev, CMU; Barry Rand, Princeton; Chris Giebink, University of Michigan) NSF, \$990,450 (CMU share), 10/01/23- 9/30/27
- “Machine Learned Potentials (MLPs) for Structure Prediction of Molecular Crystals and Interfaces” Meta, \$627,611, 02/05/24- 3/31/26
- CMU Scott Institute supplemental funding to DMREF, \$276,821, 9/01/24-8/31/27
- “Machine Learned Potentials (MLPs) for Structure Prediction of Molecular Crystals and Interfaces-Renewal 1” Meta, \$180,000 5/1/26- 4/30/27
- Co-Principal Investigator:
 - B. Hunt and N. Marom (sub-award through University of Pittsburgh), “PIRE: Hybrid Materials for Quantum Science and Engineering (HYBRID)”, NSF, \$1,188,978, 01/01/18 – 12/31/23.
 - A. McGaughey and N. Marom, “Chalcogenides for Electronic Applications”, CIT Incubation Grant, \$140,610, 09/01/18-08/31/19.
 - N. Marom (sub-award through University of Minnesota) “Integrated Materials Platforms for Topological Quantum Computing Systems”, DOE, \$368,408, 09/01/18- 08/31/21.
 - N. Marom (sub-award through University of Minnesota) “Integrated Materials Platforms for Topological Quantum Computing Systems”, DOE, \$546,950 09/01/21- 08/31/24.
 - N. Marom (sub-award through University of Minnesota) “Integrated Materials Platforms for Topological Quantum Computing Devices”, DOE, \$400,000 09/01/24- 08/31/27
 - N. Marom (sub-award through Lawrence Berkeley National Lab) “High-Fidelity AI-Ready Excited-State Materials Datasets and AI Models for Accelerated Discovery”, DOE, \$82,498 09/01/26-03/31/27

Teaching:

Carnegie Mellon University:

Electronic and Atomistic Simulation Tools (27-735)
 Engineering the Materials of the Future (27-100)
 Quantum Mechanics of Materials (27-710)

Tulane University:

Atomic and Molecular Physics (PHYS-7160)
 Quantum Mechanics I (PHYS-7170)
 Quantum Mechanics II (PHYS-7180)
 Solid State Physics (PHYS-7130)
 Modern Physics II (PHYS-2360)

Thesis Committee member:

Carnegie Mellon University:

Tong Wang, Materials Science and Engineering (research progress evaluation 12/10/25)
 Mohamed Safwat Ali, Materials Science and Engineering (research progress evaluation 5/9/25)
 Brianna Greenstein, Chemistry, University of Pittsburgh (defense 5/31/24)
 Connor Sullivan, Materials Science and Engineering (research progress evaluation 12/11/23)
 Andrew Timmins, Materials Science and Engineering (research progress evaluation 10/18/23)
 Malcolm Jardine, Physics, University of Pittsburgh (committee meeting 4/8/22, defense 7/14/23)
 Amrita Purkayastha, Physics, University of Pittsburgh (committee meeting 10/29/21)
 Jie Gong, Mechanical Engineering (thesis proposal 2/4/21, defense 5/5/21)
 Chunzhi Wu, Civil and Environmental Engineering (comprehensive exam 1/29/21)
 Joseph Pugar, Materials Science and Engineering (research progress evaluation 12/9/20)
 Yumin Zhang, Materials Science and Engineering (research progress evaluation 11/16/18)
 Xiaou Zhang, Physics (annual review 10/3/18, thesis defense 5/15/19)
 Christopher Hanselman, Chemical Engineering (proposal 1/26/17)

Tulane University:

Yang Zhang, Physics and Engineering Physics (prospectus 5/19/14)

Undergraduate Mentoring:

Vashisth Parekh (Fall 2019- Spring 2022)

Shivani Shukla (Fall 2017- Spring 2020)

Synergistic Activities:

Service to the scientific community:

- Professional society membership:
 - American Physical Society (APS)
 - American Chemical Society (ACS)
 - Materials Research Society (MRS)
 - The Minerals, Metals, and Materials Society (TMS)
 - American Crystallographic Association (ACA)
- Reviewer for **24** scientific journals of major publishers:
 - APS Journals: Physical Review B, Physical Review Letters
 - ACS Journals: Journal of Chemical Theory and Computation, Journal of Physical Chemistry, Journal of Physical Chemistry Letters, Crystal Growth & Design, ACS Applied Materials and Interfaces
 - AIP Journals: Journal of Chemical Physics, Journal of Renewable and Sustainable Energy
 - RSC Journals: Physical Chemistry Chemical Physics, Journal of Materials Chemistry, Energy & Environmental Science, Chemical Science
 - Elsevier Journals: Computational and Theoretical Chemistry, Solid State Communications, Organic Electronics
 - Wiley Journals: Physica Status Solidi B: Basic Solid State Physics, ChemPhysChem, International Journal of Quantum Chemistry, Angew. Chem.
 - Nature Journals: Nature Communications, Scientific Data, Nature Materials
 - Cambridge Core: MRS Communications
- Grant proposal reviewer:
 - NSF Condensed Matter and Materials Theory (CMMT)
 - NSF Chemical Theory, Models and Computational Methods (CTMC)
 - ACS Petroleum Research Fund (PRF)
 - Israel Science Foundation (ISF)
 - Israel Ministry of Science, Technology and Space
 - Deutsche Forschungsgemeinschaft (German Research Foundation)
 - Irish Research Council (IRC)
 - DOE Condensed Phase and Interfacial Molecular Science (CPIMS)
 - DOE Materials Science and Engineering (MSE)
 - The US-Israel Binational Science Foundation (BSF)
 - DOE Advanced Scientific Computing Research (ASCR)
 - DOE Established Program to Stimulate Competitive Research (EPSCoR)
 - NSF Designing Materials to Revolutionize and Engineer our Future (DMREF)
- Computer time proposal reviewer:
 - The Brookhaven Center for Functional Nanomaterials (CFN)
 - Cy-Tera, the Cyprus Institute high performance computing facility
 - The Argonne Center for Nanoscale Materials (CNM)
 - The Partnership for Advanced Computing in Europe (PRACE)
 - CSCS Swiss National Supercomputing Centre
- Expert reviewer for tenure track applications or promotions at:
 - Argonne National Laboratory
 - Technical University Munich, Germany

- Organizer:
 - Focus Session “Van der Waals Interactions in Advanced Materials”, The 2015 Meeting of the American Physical Society, San Antonio, TX, USA, 03/’15.
 - Telluride Science Research Center (TSRC) workshop “Multiscale Simulations of Organic Electronic Materials” Telluride, CO, USA, 07/’15.
 - Symposium 4A: “Advances in Computational Materials Science”, XXIV International Materials Research Congress (IMRC), Cancun, Mexico, 08/’15.
 - Focus Session “Many-Body Perturbation Theory for Electronic Excitations in Materials”, The 2016 Meeting of the American Physical Society, Baltimore, MD, USA, 03/’16.
 - “Workshop III: Collective Variables in Quantum Mechanics” within The UCLA Institute for Pure and Applied Mathematics (IPAM) long program “Understanding Many-Particle Systems with Machine Learning”, Los Angeles, CA, 11/’16.
 - Focus Session “First Principles Modeling of Excited State Phenomena in Materials”, The 2017 Meeting of the American Physical Society, New Orleans, LA, USA, 03/’17.
 - The UCLA Institute for Pure and Applied Mathematics (IPAM) long program “Complex High-Dimensional Energy Landscapes”, and “Workshop I: Optimization and Optimal Control for Complex Energy and Property Landscapes”, Los Angeles, CA, USA, 09’-12/’17.
 - Focus Session “First Principles Modeling of Excited State Phenomena in Materials”, The 2018 March Meeting of the American Physical Society, Los Angeles, CA, USA, 03/’18.
 - “Fundamental Science 4: Optical Excitations and Ultrafast Phenomena in Condensed Matter” 2018 CLEO Conference and Exhibition (Laser Science to Photonic Applications), San Jose, California, USA, 05/’18.
 - Symposium D1: “Computational Discovery of Advanced Materials”, XXVII International Materials Research Congress (IMRC), Cancun, Mexico, 08/’18.
 - The UCLA Institute for Pure and Applied Mathematics (IPAM) workshop “Quantum Computing Materials Challenges (QCM)”, Los Angeles, CA, USA, 08/’18.
 - The UCLA Institute for Pure and Applied Mathematics (IPAM) workshop “Theory and Computation for 2D Materials”, Los Angeles, CA, USA, 01/’20.
 - Focus Session “Van der Waals Interactions in Molecules, Materials, and Complex Environments”, The 2020 Meeting of the American Physical Society, Denver, CO, USA, 03/’20 (cancelled due to COVID).
 - DCOMP Program Committee member, The 2020 March Meeting of the American Physical Society, Denver, CO, USA, 03/’20 (cancelled due to COVID).
 - Focus Session “Van der Waals Interactions in Molecules, Materials, and Complex Environments”, The 2021 March Meeting of the American Physical Society, 03/’21 (virtual).
 - PHYS symposium “Crystalline Organic Electronics and Photonics-Theory and Experiment”, the American chemical Society (ACS) Spring 2026 Meeting, 03/’26.
- Session Chair:
 - Symposium O “Computational modelling of organic semiconductors: from the quantum world to actual devices”, Session O.4 “Electronic Structure of Molecular Solids”, European Materials Research Society (E-MRS) 2014 Spring Meeting, Lille, France, 05/’14.
 - Session L16 “Focus Session: van der Waals Bonding in Advanced Materials: Molecular Systems and Interfaces”, 2015 March Meeting of the American Physical Society, San Antonio, TX, USA, 03/’15.
 - “Density Functional Theory” session, Multiscale Simulations of Organic Electronic Materials, Telluride, CO, USA 07/’15.
 - Symposium 4A: “Advances in Computational Materials Science”, XXIV International Materials Research Congress (IMRC), Cancun, Mexico 08/’15.
 - Session P24 “Many-Body Perturbation Theory for Electronic Excitations: Electronic Structure”, 2016 March Meeting of the American Physical Society, Baltimore, MD, USA, 03/’16.
 - “Understanding Many-Body Systems with Machine Learning I: Machine Learning Meets Many-Particle Problems”, Los Angeles, CA 09/’16.
 - Session “General IV” EMN Meeting on Computation and Theory 2016, Las Vegas, NV 10/’16.
 - “Understanding Many-Body Systems with Machine Learning III: Collective Variables in Quantum Mechanics”, Los Angeles, CA 11/’16.

- Plenary 6 “Quantum Materials and Spectroscopy” 57th Sanibel Symposium, St. Simons Island, GA, USA 02/’17.
- Session B1 “Computational Discovery and Design of Novel Materials II”, 2017 March Meeting of the American Physical Society, New Orleans, LA USA, 03/’17.
- Session K7 “First-Principles Modeling of Excited State Phenomena IV: Molecular Systems and Singlet Fission”, 2017 March Meeting of the American Physical Society, New Orleans, LA USA, 03/’17.
- Session E29 “First-principles Modeling of Excited-State Phenomena in Materials IV: Nanoscale Systems”, 2018 March Meeting of the American Physical Society, Los Angeles, CA USA, 03/’18.
- Session GI01.06: “Machine Learning for Imaging, Characterization and Inverse Problems”, 2018 Materials Research Society Fall Meeting, Boston, MA, USA, 11/’18.
- Session B19 “Van Der Waals Interactions in Molecules, Materials, and Complex Environments II” The 2021 March Meeting of the American Physical Society, 03/’21 (virtual).
- “2D Materials for Energy, Sensing and Quantum Information Science: Computation & 2D general” 2021 Spring Meeting of the American Chemical Society, virtual, 04/’21.
- Editorial roles:
 - **Associate Editor, npj Computational Materials**, *impact factor 9.7* (2022 – present)
 - The Journal of Chemical Physics Editorial Advisory Board (2021- present)
 - Guest Editor, the Journal of Chemical Physics Special Issue on Computational Materials Discovery
- Board membership:
 - The Argonne Leadership Computing Facility (ALCF) User Advisory Council (2016-2020)
 - PIRE: Hybrid Executive Committee (2017-2022)
 - International Conference on the Chemistry of the Organic Solid State (ICCOSS) Advisory Board (2019- 2022)
 - FHI-aims Advisory Group (2019- present)
 - Cambridge Crystallographic Data Centre (CCDC) Crystal Structure Prediction (CSP) Working Group (2019- present)
- Faculty mentoring:
 - Panelist at the CIT Center for Faculty Success NSF CAREER workshop (2019, 2020)
 - Panelist at the CMU Rising Stars Workshop (2023)
- Other:
 - Poster judge at The 2015 Southeastern Theoretical Chemistry Association (SETCA) Annual Meeting, Orlando, FL, USA 05/’15.

Service to the Materials Science and Engineering Department at Carnegie Mellon:

- Graduate teaching intern award selection (Fall 2024-Fall 2025)
- Chair of the MSE IT Ad Hoc Committee (Fall 2022- Spring 2023)
- Organizer of the departmental seminar series (Spring 2021- present)
- Member of the Graduate Curriculum Committee (Spring 2019- Spring 2020)
- Member of the Computational MS Program Ad Hoc Committee (Fall 2018)
- Member of the Diversity Committee (Spring 2018- Spring 2020)
- Member of the Undergraduate Curriculum Committee (Fall 2016- Spring 2020)

Service to the College of Engineering at Carnegie Mellon:

- Member of the CIT Reappointment Promotion and Tenure (RPT) Ad Hoc Committee (Fall 2025-present)
- Member of the CIT Computing Committee (Spring 2019- Spring 2020)

Service to the Physics and Engineering Physics Department at Tulane:

- Founder and Chair of the Diversity Committee (Summer 2014- Spring 2016)

- Member of the Materials Engineering PhD Program Committee (Fall 2013- Spring 2016)
- Member of Graduate Recruitment and Admissions Committee (Fall 2013- Spring 2016)
- Member of Theory Faculty Search Committee (Fall 2013- Spring 2014)
- Chair of the Newsletter and Publicity Committee (Fall 2013- Spring 2014)

Service to Tulane University:

- Member of The Senate Information Technology (IT) Committee (Fall 2013-Spring 2016)

Broadening the participation of underrepresented groups in science:

- Co-organizer of “Womanhood” activities (for advancing women in science) at the Weizmann Institute of Science (2007-2010)
- Speaker at a meeting of the Penn State “Physics and Astronomy Women (PAW)” student group, 12/’12
- Fellow of the Newcomb College Institute at Tulane (Fall 2013-Spring 2016)
- Streaming the “Atomic and Molecular Physics” graduate course to other institutions in Louisiana including historically black colleges and universities (HBCUs) within the Louisiana Alliance for Simulation Guided Materials Applications (LA-SiGMA), Spring 2014
- Organizer of the “Women Leaders in Physics and Engineering” colloquium series at Tulane (Fall 2014-Spring 2016)
- Speaker at a meeting of the Tulane “Women in Science (WIS)” student group, 09/’14
- Speaker at a meeting of the University of Central Florida “Women Physics Students (WPS)” group, 04/’15
- Speaker at a meeting of the Penn State “Physics and Astronomy Women (PAW)” student group, 01/’17
- Organizer of the “Women Leaders in Science and Engineering” (WLSE) events at Carnegie Mellon (Fall 2016- present)