Curriculum Vitae:
Sivan Refaely-Abramson

Senior Scientist,
Dept. of Materials and Interfaces,
Weizmann Institute of Science, Israel

December 2019

Personal details

Date of Birth: March 26, 1982
Country of Birth: Israel
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Education

2004 - 2007: **Bachelor's degree** at the Hebrew University of Jerusalem, within the Exact Sciences Combined Honors Program (Chemistry and Physics), magna cum laude.

2009 - 2011: **Master's degree** at the Weizmann Institute of Science. Supervisor: Prof. Leeor Kronik; Title of thesis: "Excitation gaps in organic molecules from an optimally tuned range-separated hybrid functional".

2011 - 2015: **Doctorate- direct track** at the Weizmann Institute of Science. Supervisor: Prof. Leeor Kronik; Title of thesis: "A generalization of the optimally-tuned range-separated hybrid scheme to the solid-state".

2015 - 2018: **Postdoctoral fellow** at the Physics Department, University of California, Berkeley; Molecular Foundry, Lawrence Berkeley National Laboratory; and the Center for Computational Study of Excited-State Phenomena in Energy Materials (C2SEPEM), Berkeley. Host: Prof. Jeffrey B. Neaton. Research area: advanced first-principles calculations of excited state phenomena in complex systems.

2018 - present: **Senior Scientist** at the Department of Materials and Interfaces, Weizmann Institute of Science, Israel.

Scholarships and Awards

- Alon Fellowship for young faculty members, awarded by the Israeli Council for Higher Education (2019).
- Peter and Patricia Gruber Award for Young Scientists at the Weizmann Institute (2019).
- Rothschild Foundation Post-Doctoral Fellowship (2015-2016).
- Fulbright - Ilan Ramon Post-Doctoral Fellowship (2015-2016).
- National Postdoctoral Award for Advancing Women in Science (2015-2016).
- Israel Chemical Society Excellent Graduate Student Prize (2016).
- Dov Elad Memorial Feinberg Graduate School Award for Outstanding Ph.D. Research (2015).
- Adams Fellowship Award for Outstanding Ph.D. Students of the Sciences (2013-2015).
- Best Lecture Award at the Student Conference on Solar Energy, Weizmann Institute of Science (2013).
- Best Student Poster Award at the 7th International Workshop on Electronic Structure and Processes at Molecular-Based Interfaces (2013).
- Feinberg Graduate School Excellence Award for M.Sc. Students (2012).
- Dean's List in the Faculty of Exact Sciences, the Hebrew University of Jerusalem (2007).
- Orion Scholarship for high achievements, the Hebrew University of Jerusalem (2006).
- Dean's List in the Faculty of Exact Sciences, the Hebrew University of Jerusalem (2005).

Grants

2020 - 2023: Minerva Foundation Research Grant, granted September 2019.
2019 - 2023: Israel Science Foundation Personal Grant, granted July 2019.

2019 - 2023: Israel Science Foundation Equipment Grant, granted July 2019.

2019 - 2021: US-Israel Binational Science Foundation Startup Grant, granted July 2019.
2019 - 2020: Molecular Foundry User research Grant, granted May 2019.

List of Publications

1. B. Schuler, J-H. Lee, C. Kastl, K. Cochrane, C. Chen, S. Refaely-Abramson, S. Yuan, E. van Veen,R. Roldan, N. Borys, R. Koch, S. Aloni, A. Schwartzberg, F. D. Ogletree,J. B. Neaton, A. Weber-Bargioni, "How Substitutional Point Defects in Two-Dimensional WS2 Induce Charge Localization, Spin-Orbit Splitting, and Strain", *ACS Nano* **13**, 10520-10534 (2019)

2. B. Schuler, D. Y. Qiu, S. Refaely-Abramson , C. Kastl, C. T. Chen, S. Barja, Roland J. Koch, D. F. Ogletree, S. Aloni, A. M. Schwartzberg, J. B. Neaton, S. G. Louie, and A. Weber-Bargioni, "Large spin-orbit splitting of deep in-gap defect states of engineered sulfur vacancies in monolayer WS_2", *Phys. Rev. Lett.* **123**, 076801 (2019)

3. S. Barja†, S. Refaely-Abramson†, B. Schuler, D. Y. Qiu, A. Pulkin, S. Wickenburg, H. Ryu, M. M. Ugeda, C. Kastel, C. Chen, C. Hwang, A. M. Schwarzburg, S. Aloni, S.-K. Mo, D. F. Ogletree, M. F. Crommie, O. Yazyev, S. G. Louie, J. B. Neaton, and A. Weber-Bargioni, "Identifying substitutional oxygen as a prolific point defect in monolayer transition metal dichalcogenides with experiment and theory", *Nature Comm.* **10**, 3382 (2019)

4. S. Refaely-Abramson, Z.-F. Liu, F. Bruneval, and J. B. Neaton, "First-Principles Approach to the Conductance of Covalently Bound Molecular Junctions" *J. Phys. Chem. C* **123**, 11, 6379-6387 (2019)

5. S. Refaely-Abramson†, D. Y. Qiu†, S. G. Louie, and J. B. Neaton, "Defect-induced modification of low-lying excitons and valley selectivity in monolayer transition metal dichalcogenides", *Phys. Rev. Lett.* **121**, 167402 (2018)

6. J. Brisendine†, S. Refaely-Abramson†, Z.-F. Liu†, J. Cui, F. Ng, J. B. Neaton, R. Koder, and L. Venkataraman, "Probing Charge Transport through Peptide Bonds", *J. Phys. Chem. Lett.* **9**, 763-767 (2018)

7. B. D. Folie, J. B. Haber, S. Refaely-Abramson, J. B. Neaton and N. S. Ginsberg, "Long-Lived Correlated Triplet Pairs in a π-Stacked Crystalline Pentacene Derivative", *J. Am. Chem. Soc.* **140**, 2326-2335 (2018)

8. C. Guo, S. Sarkar, S. Refaely-Abramson, D. A. Egger, T. Bendikov, K. Yonezawa, Y. Suda, T. Yamaguchi, I. Pecht, S. Kera, N. Ueno, M. Sheves, L. Kronik, D. Cahen, "Electronic structure of dipeptides in the gas-phase and as an adsorbed monolayer", *Phys. Chem. Chem. Phys.* **20**, 6860-6867 (2018)

9. A. Manna, S. Refaely-Abramson, A. M. Reilly, A. Tkatchenko, J. B. Neaton, and L. Kronik, "Quantitative prediction of optical absorption in molecular solids from an optimally-tuned screened range-separated hybrid functional", *J. Chem. Theory Comput.* **14**, 2919-2929 (2018)

10. S. Refaely-Abramson†, F. H. da Jornada†, S. G. Louie, and J. B. Neaton, "Origins of singlet fission in solid pentacene from an ab initio Green's-function approach", *Phys. Rev. Lett.* **119**, 267401 (2017)

11. Z.-F. Liu, D. A. Egger, S. Refaely-Abramson, L. Kronik, and J. B. Neaton, "Energy level alignment at molecule-metal interfaces from an optimally-tuned range-separated hybrid functional", *J. Chem. Phys.* **146**, 092326 (2017)

12. C. Guo, X. Yu, S. Refaely-Abramson, L. Sepunaru, T. Bendikov, I. Pecht, L. Kronik, A. Vilan, M. Sheves, and D. Cahen, "Tuning electronic transport via hepta-alanine peptides junction by tryptophan doping", *Proc. Natl. Acad. Sci. USA* **113**, 10785-10790 (2016)

13. M. Eckshtain-Levi†, E. Capua, S. Refaely-Abramson†, S. Sarkar†, Y. Gavrilov, S. P. Mathew, Y. Paltiel, Y. Levy, L. Kronik, and R. Naaman, "Cold denaturation induces inversion of dipole and spin transfer in chiral peptide monolayers", *Nature Comm.* **7**, 10744 (2016)

14. S. Refaely-Abramson, M. Jain, S. Sharifzadeh, J. B. Neaton, and L. Kronik, "Solid-state optical absorption from optimally tuned time-dependent range-separated hybrid density functional theory", *Phys. Rev. B (Rapid Comm.)* **92**, 081204 (2015)

15. L. Sepunaru, S. Refaely-Abramson, R. Lovrincic, Y. Gavrilov, P. Agrawal, Y. Levy, L. Kronik, I. Pecht, M. Sheves, D. Cahen, "Electronic transport via homo-peptides: The role of side chains and secondary structure", *J. Am. Chem. Soc.* **137**, 96179626 (2015)

16. D. A. Egger, S. Weismann, S. Refaely-Abramson*, S. Sharifzadeh, M. Dauth, R. Baer, S. Kmmel, J. B. Neaton, E. Zojer, and L. Kronik*, "Outer-valence electron spectra of prototypical aromatic heterocycles from an optimally-tuned range-separated hybrid functional", *J. Chem. Theory Comput.* **10**, 1934-1952 (2014)

17. I. Tamblyn, S. Refaely-Abramson, J. B. Neaton, and L. Kronik, "Simultaneous determination of structures, vibrations, and frontier orbital energies from a self-consistent range-separated hybrid functional", *J. Phys. Chem. Lett.* **5**, 2734-2741 (2014)

18. D. Lüftner, S. Refaely-Abramson, M. Pachler, R. Resel, M. G. Ramsey, L. Kronik, and P. Puschnig, "Experimental and theoretical electronic structure of quinacridone", *Phys. Rev. B* **90**, 075204 (2014)

19. S. Refaely-Abramson, S. Sharifzadeh, M. Jain, R. Baer, J. B. Neaton, and L. Kronik, Gap renormalization of molecular crystals from density functional theory, Phys. Rev. B (Rapid Comm.) 88, 081204-1/5(RC) (2013)

20. S. Refaely-Abramson, S. Sharifzadeh, N. Govind, J. Autschbach, J. B. Neaton, R. Baer, and L. Kronik, "Quasiparticle spectra from a non-empirical optimally-tuned range separated hybrid density functional", *Phys. Rev. Lett.* **109**, 226405 (2012)

21. L. Kronik, T. Stein, S. Refaely-Abramson, and R. Baer, "Excitation gaps of finite-sized systems from optimally-tuned range- separated hybrid functionals", *J. Chem. Theory Comput.* **8**, 1515-1531 (2012)

22. S. Refaely-Abramson, R. Baer and L. Kronik, "Fundamental and excitation gaps in molecules of relevance for organic photovoltaics from an optimally tuned range-separated hybrid functional", *Phys. Rev. B* 84, 075144 (2011), **Editor's Suggestion**.

* Corresponding author
† Joint first author

Presentations

Invited Lectures

1. ”Complex Exciton Phenomena in Functional Materials from many-body perturbation theory”, Israel-Italy Workshop on 2D Materials, Bar Ilan University, November 2019.
2. ”Computing Excited States in Functional Materials using Many-Body Perturbation Theory”, Photo and Electro-Catalysis at the Atomic Scale (PECAS 2019), Donostia International Physics Center (DIPC), Donostia-San Sebastián, Spain, August 2019.
3. ”First Principles Approach to the Conductance of Covalently Bound Molecular Junctions”, Quantum transport in nanoscale molecular systems workshop, Telluride, CO, USA, July 2019.
4. ”Exciton Phenomena in Molecular Crystals: Effect of Structure and Symmetry”, the 3rd Israeli Conference on Computational Modeling of Molecules and Solids, Ben-Gurion University of the Negev, Israel, July 2019.
5. ”Multiexciton Generation Processes in Organic Crystals from First-Principles”, the 84th Israel Chemical Society Meeting, Tel-Aviv, Israel, February 2019.
6. ”Effect of point defects in TMDs: a computational perspective”, Winter School on 2D Materials, Weizmann Institute of Science, Rehovot, Israel, January 2019.
7. ”Exciton Interactions in Crystals from Many-Body Perturbation Theory”, The Isaiah Shavitt Workshop Series, Technion, Haifa, Israel, January 2019.
8. ”Charge transport through peptides: a computational perspective”, the BIOMOLECTRO conference, Madrid, Spain, August 2018.
9. ”New Insights into Single- and Multi-Exciton Phenomena in Complex Materials from Ab Initio Many-Body Perturbation Theory”, the American Physical Society March Meeting, Los-Angeles, CA, USA, March 2018.
10. ”Single- and Multi-Exciton Phenomena in Organic Systems from First Principles: The Case of Singlet-Fission in Molecular Crystals”, the 254th American Chemical Society National Fall Meeting, Washington, DC, USA, August 2017.
11. ”Excited-State Phenomena in Molecular Solids from First Principles”, NG-NEXT workshop, Los-Angeles, CA, USA, October 2016.
12. ”Solid-State Optical Absorption from Optimally-Tuned Time-Dependent Screened Range-Separated Hybrids”, the 7th Time-Dependent Density-Functional Theory Prospects and Applications, Benasque, Spain, September 2016.
13. ”Predicting Solid State Excitations using Density Functional Theory”, the 28th annual workshop on recent developments in electronic structure methods, Albuquerque, NM, USA, June 2016.
14. ”Quantitative photoelectron and optical spectroscopy of organic electronic materials from optimally-tuned range-separated hybrid density functional theory”, the Penn Conference on Theoretical Chemistry - Theory of Energy Conversion, University of Pennsylvania, Philadelphia, PA, USA, July 2015.

Seminars and Colloquia

1. ”Structural effects on exciton phenomena in transition metal dichalcogenides from many-body perturbation theory”, 2D Materials Seminar, Stanford University, CA, USA, August 2019.
2. ”Structural Effects on Complex Excited-State Phenomena in 2D and Molecular Crystals”, Max Planck Institute at Hamburg, Germany, May 2019.
3. ”Excitons and Symmetry: Structural Effects on Complex Excited-State Phenomena in 2D and Molecular Crystals”, SFB - Topical Seminar at the University of Regensburg, Germany, May 2019.
4. ”Structural Effects on Complex Excited-State Phenomena in Molecular Crystals”, University of Cambridge, UK, May 2019.
5. ”Complex Excitonic Phenomena in Photophysics from Advanced Computational Approaches”, Condensed Matter Physics Seminar, Weizmann Institute of Science, Rehovot, Israel, April 2019.
6. ”Complex Excited-State Phenomena from Predictive Computational Approaches”, Boston University, USA, September 2018.
7. ”Complex Excitonic Interactions in Photophysics from Advanced Computational Approaches”, Donostiarra International Physics Center, San Sebastián, Spain, August 2018.
8. ”Complex Excitonic Interactions in Photophysics from Advanced Computational Approaches”, Applied Physics Departmental seminar, the Hebrew University of Jerusalem, Israel, June 2018.
9. ”New Insights into Complex Excited-State Phenomena from Predictive Computational Approaches”, Physical Chemistry Departmental seminar, the Hebrew University of Jerusalem, Israel, May 2018.
10. ”New Insights into Complex Excited-State Phenomena from Predictive Computational Approaches”, School of Chemistry at the Technion, Israel, May 2018.
11. ”New Insights into Complex Excited-State Phenomena from Predictive Computational Approaches”, Faculty of Engineering, Bar-Ilan University, Israel, May 2018.
12. ”New Insights into Complex Excited-State Phenomena from Predictive Computational Approaches”, Chemistry Departmental seminar at the Weizmann Institute of Science, March 2018.
13. ”New Insights into Complex Excited-State Phenomena from Predictive Computational Approaches”, Chemistry Departmental seminar at the Tel Aviv University, March 2018.
14. ”Predicting Electronic Properties of Materials for Photovoltaics using New Approaches within Density Functional Theory”, Physical Chemistry Departmental seminar at the Hebrew University of Jerusalem, June 2015.

Contributed Oral Presentations

1. ”Complex Exciton Phenomena in Functional Materials from many-body perturbation theory”, Psi-k - CECAM conference on Ultrafast Physics from Molecules to Nanostructures, Donostia-San Sebastián, Spain,, October 2019.

2. ”Complex Excited-State Phenomena in 2D and Molecular Crystals: Effects of Structure and Symmetry”, the Weizmann-India Exchange Conference, Weizmann Institute of Science, Israel, May 2019.

3. ”Structural Effects on Excitonic Phenomena in Organic Crystals”, the American Physical Society March Meeting, Boston, MA, USA, March 2019.

4. ”Excited State Phenomena in Molecular Crystals from Many-Body Perturbation Theory”, Structural and electronic dynamics in soft semiconductors workshop, Weizmann Institute of Science, Israel, February 2019.

5. ”Structural Effects on Excited-State Phenomena: A Computational Perspective”, WISCIT Workshop on Novel Materials, Caltech Institute of Science, CA, USA, November 2018.

6. ”Harnessing Energy with Symmetry”, the 2018 Rothschild Fellows Colloquium, Jerusalem, Israel, May 2018.

7. ”Singlet Fission in Solid Pentacene from First Principles”, the 2017 Singlet-Fission Workshop, Lyons, CO, USA, June 2017.

8. ”Singlet-Fission from First-Principles Many-Body Perturbation Theory”, the American Physical Society March Meeting, New Orleans, LA, USA, March 2017.

9. ”Exciton Coupling from GW-BSE: The Case of Singlet-Fission”, the NSF-MolSSI Sponsored Workshop on Materials Software, Berkeley, CA, USA, February 2017.

10. ”Predicting Excitons in Molecular Solids from First Principles: Advances in Computational Methods”, the 2016 Singlet-Fission Workshop, Lyons, CO, USA, June 2016.

11. ”Solid-State Optical Absorption from Optimally-Tuned Time-Dependent Range-Separated Hybrid DFT”, the American Physical Society March Meeting, Baltimore, MD, USA, March 2016.

12. ”Cold denaturation induces inversion of dipole and spin transfer in chiral peptide monolayers, the American Physical Society March Meeting, Baltimore, MD, USA, March 2016.

13. ”Predicting spectroscopic properties of organic molecules and crystals using density functional theory”, Frontiers in Chemical Science international symposium at the Weizmann Institute of Science, Rehovoth, Israel, May 2015.

14. ”Theoretical and Experimental Electronic Structure of Quinacridone”, the American Physical Society March Meeting, San-Antonio, TX, USA, March 2015.

15. ”Spectroscopic predictions of organic systems from density functional theory”, Quantum Theory and Multi-Scale Modeling for Energy Applications, University of Pennsylvania, Philadelphia, PA, USA, March 2015.

16. ”Gap renormalization and outer-valence spectra in molecular crystals”, Mini-symposium on electronic structure and dynamics, Rehovoth, Israel, December 2014.

17. ”Gap renormalization of molecular crystals from density functional theory”, the European Materials Research Society Meeting, Lille, France, May 2014.

18. ”Gap renormalization of molecular crystals from density functional theory”, the American Physical Society March Meeting, Denver, CO, USA, March 2014.

19. ”Gap renormalization of molecular crystals from density functional theory”, the 16th Israel Materials Engineering Conference, Haifa, Israel, February 2014.

20. ”Spectroscopic predictions of organic systems from density functional theory”, the 2013 Student Conference on Solar Energy, Rehovoth, Israel, December 2013, received the Best Lecture Award.

21. ”Predicting band-gaps and photoemission spectra using density functional theory”, the annual meeting of the Israel Science Foundation, Rehovoth, Israel, November 2013.

22. ”Quasi-particle spectra and gap renormalization from density functional theory”, the annual meeting of the Lise Meitner Computational Chemistry Center, Rehovoth, Israel, November 2013.

23. ”Fundamental gaps and photoemission spectra from ground-state DFT”, the Gordon Research Seminar on Time-Dependent Density-Functional Theory, Biddeford, ME, USA, August 2013.

24. ”Quasiparticle-level spectra from DFT with an optimally-tuned range-separated hybrid functional”, From Density Functional Theory principles to material properties workshop, Bayreuth, Germany, September 2012.

25. ”Fundamental and excitation gaps in molecules of relevance for organic photovoltaics from an optimally tuned range-separated hybrid functional”, The American Physical Society March Meeting, Boston, MA, USA, February 2012.

26. ”Fundamental and excitation gaps in molecules of relevance for organic photovoltaics”, the 57th Annual Meeting of the Israel Physical Society, Haifa, Israel, December 2011.

Posters

1. ”The C2SEPEM computational center: Validation, Verification, and Applications”, 2018 DOE Mid-Review, Washington DC, USA, June 2018.
2. ”Effects of molecular packing in organic crystals on singlet fission with ab initio many body perturbation theory”, 2017 EFRC-Hub-CMS PI meeting, Washington DC, USA, July 2017.
3. ”Electronic structure of homopeptides and its relation to transport”, Batsheva de Rothschild Seminar on Molecular Electronics, Ma’ale Hachamisha, Israel, June 2015.
4. ”Solid-state excitonic effects predicted from optimally-tuned time-dependent range separated hybrid density functional theory”, Ma’ale Hachamisha, Israel, June 2015.
5. ”Solid-state excitonic effects predicted from optimally-tuned time-dependent range separated hybrid density functional theory”, Lise Meitner Minerva Symposium, Tel Aviv University, Tel Aviv, Israel, May 2015.
6. ”Simultaneous determination of structures, vibrations, and frontier orbital energies from a self-optimizing range-separated hybrid functional”, COST meeting on fundamental problems in quantum mechanics, Rehovoth, Israel, March 2014.
7. ”Quasiparticle Spectra and gap renormalization from density functional theory”, CECAM workshop: Quantum dynamics in molecular and nano-materials: mechanics and functionality, Tel-Aviv, Israel, November 2013.
8. ”Quasiparticle Spectra and gap renormalization from density functional theory”, the Gordon Research Conference on Time-Dependent Density-Functional Theory, Biddeford, ME, USA, August 2013.
9. ”Quasiparticle spectra from a non-empirical optimally-tuned range separated hybrid density functional”, 7th International Workshop on Electronic Structure and Processes at Molecular-Based Interfaces (ESPMI VII), Rehovoth, Israel, May 2013, received the Best Student Poster Award.
10. ”Quasiparticle spectra from a non-empirical optimally-tuned range separated hybrid density functional”, 58th Annual Meeting of the Israel Physical Society, Jerusalem, Israel, December 2012.
11. ”Quasiparticle spectra from a non-empirical optimally-tuned range separated hybrid density functional”, Molecular Electronics International Meeting, Jerusalem, Israel, July 2012.
12. ”Fundamental and excitation gaps in molecules of relevance for organic photovoltaics from an optimally tuned range-separated hybrid functional”, 77th Annual Meeting of the Israel Chemical Society, Ramat-Gan, Israel, February 2012.