Emmanouil Semidalas

Curriculum Vitae

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Work address: Weizmann Institute of Science, Herzl 234, Rehovot, Israel
Date of birth: 18/12/1996
Nationality: Greek
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Education

17/2/2021–20/8/2024 **Ph.D. degree**, Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Rehovot, Israel

Ph.D. Thesis: Accurate and efficient composite wavefunction theory methods through localized natural orbitals and F12 explicit correlation. Supervisor: **Prof. Jan M. L. (Gershom) Martin**

Ph.D. Thesis Defense Date: 20/8/2024

19/1/2019–17/2/2021 **M.Sc. degree**, Department of Organic Chemistry, Weizmann Institute of Science, Rehovot, Israel

M.Sc. thesis: Accurate and efficient composite wavefunction theory methods through localized natural orbitals and F12 explicit correlation. Supervisor: **Prof. Jan M. L. (Gershom) Martin**

M.Sc. thesis grade: 96/100, M.Sc. thesis defense grade: 94/100

12/2/2018 – 9/3/2018 **Visiting scientist**, Advanced Amorphous Materials and Nanomaterials Lab, Institute of Chemical Engineering Sciences and Foundation for Research and Technology-Hellas, Patras, Greece

I studied the structural and electronic properties of amorphous chalcogenide and rare-earth YAG glass semiconductors using Raman, IR, and UV-vis spectroscopies, alongside quantum mechanical calculations. Supervisors: **Profs. Athanasios Chrissanthopoulos** and **Spyros Yannopoulos**

18/9/2014–28/2/2018 **B.Sc. Chemistry**, Department of Chemistry, National and Kapodistrian University of Athens, Panepistimioupoli (University Campus), Athens, Greece

B.Sc. grade: 8.8/10 (Excellent), valedictorian, graduated in 7 semesters by taking extra courses each term, B.Sc. thesis: Computational study of the structural, electrical, and vibrational properties of M_4S_6 (M = P, As, Sb, Bi) compounds, Supervisor: **Prof. Athanasios Chrissanthopoulos**, B.Sc. thesis grade: 10/10.

2/7/2014 **High School Diploma**, 67th Lyceum, Athens, Grade: 19.5/20 (Excellent)

International Summer Schools

27/8/2023–2/9/2023 **Modern Wavefunction Based Methods in Electronic Structure Theory School**, University of Pisa, Pisa, Italy. Organizers: **Profs. Jürgen Gauss** and **Frank Neese**

1/6/2017– **Kupcinet-Getz summer school**, Weizmann Institute of Science, Rehovot, Israel

1/8/2017 Interned with **Prof. Gideon Schreiber** in the Department of Biomolecular Sciences

Awards and Scholarships

1/1/2022–1/8/2024: Feinberg Graduate School Fellowship and Onassis Foundation Scholarship for Ph.D. studies

1/1/2019–1/10/2021: Feinberg Graduate School Fellowship and Onassis Foundation Scholarship for M.Sc. studies

12/8/2014: Prize award (800 EUR) for highest score in Greek University entrance exams by EUROBANK bank

3/4/2012: 3rd prize in the 72nd Panhellenic High-Schoool Mathematical Competition Euclid

Language Skills

Language	**Reading**	**Writing**	**Speaking**
Greek	Native	Native	Native
English	Fluent	Fluent	Fluent
French	Basic	Basic	Basic
Hebrew	Basic	Basic	Basic

Computer Skills

- Programming languages: Python, C, C++, Fortran
- Molecular electronic structure software: Gaussian, Molpro, MRCC, Orca, Psi4, CFOUR, Turbomole
- Molecular dynamics software: Amber and Gromacs

Publications (as of September 2024)

Total publications: 21

18 in international peer-reviewed journals, 3 in conference proceedings, 1 chapter in a scientific book

1 book translation

Number of citations: 164, h-index: 7 (Web of Science, 4/9/2024)

Publications in International Peer-Reviewed Journals

(17) Fishman V.; **Semidalas, E.**; Martin, J. M. L., "Basis Set Extrapolation from the Vanishing Counterpoise Correction Condition" *Journal of Physical Chemistry A* **2024** *in press*

(16) **Semidalas, E.**; Karton, A.; Martin, J. M. L., "W4Λ: Leveraging Λ Coupled-Cluster for Accurate Computational Thermochemistry Approaches" *Journal of Physical Chemistry A* **2024**, 128, 1715–1724 [Editor's choice]

(15) **Semidalas, E.**; Martin, J. M. L., "Can G4-like Composite *Ab Initio* Methods Accurately Predict Vibrational Harmonic

Frequencies?" *Molecular Physics* **2023**, 122, e2263593. [Tim Lee Memorial Issue]

(14) **Semidalas, E.**; Martin, J. M. L., "Correlation Consistent Basis Sets for Explicitly Correlated Theory: The Transition Metals" *Journal of Chemical Theory and Computation* **2023**, 19, 5806–5820.

(13) Spiegel, M.; **Semidalas, E.**; Martin, J. M. L.; Bentley, M. R.; Stanton, J. F., "Post-CCSD(T) Corrections to Bond Distances and Vibrational Frequencies: The Power of Λ" *Molecular Physics* **2023**, 122, e2252114. [Tim Lee Memorial Issue]

(12) **Semidalas, E.**; Martin, J. M. L., "The MOBH35 Metal–Organic Barrier Heights Reconsidered: Performance of Local-Orbital Coupled Cluster Approaches in Different Static Correlation Regimes" *Journal of Chemical Theory and Computation* **2022**, 18, 883–898.

(11) **Semidalas, E.**; Martin, J. M. L., "Automatic Generation of Complementary Auxiliary Basis Sets for Explicitly Correlated Methods" *Journal of Computational Chemistry* **2022**, 43, 1690–1700.

(10) Santra, G.; **Semidalas, E.**; Mehta, N.; Karton, A.; Martin, J. M. L. "S66×8 Noncovalent Interactions Revisited: New Benchmark and Performance of Composite Localized Coupled-Cluster Methods" *Physical Chemistry Chemical Physics* **2022**, 24, 25555–25570.

(9) Santra, G.; **Semidalas, E.**; Martin, J. M. L., "Surprisingly Good Performance of XYG3 Family Functionals Using a Scaled KS-MP3 Correlation" *Journal of Physical Chemistry Letters* **2021**, 12, 9368–9376.

(8) Santra, G.; **Semidalas, E.**; Martin, J. M. L., "Exploring Avenues beyond Revised DSD Functionals: II. Random-Phase Approximation and Scaled MP3 Corrections" *Journal of Physical Chemistry A* **2021**, 125, 4628–4638.

(7) **Semidalas, E.**; Martin, J. M. L., "Canonical and DLPNO-Based Composite Wavefunction Methods Parametrized against Large and Chemically Diverse Training Sets. 2: Correlation-Consistent Basis Sets, Core–Valence Correlation, and F12 Alternatives" *Journal of Chemical Theory and Computation* **2020**, 16, 7507–7524.

(6) **Semidalas, E.**; Martin, J. M. L., "Canonical and DLPNO-Based G4(MP2)XK-Inspired Composite Wave Function Methods Parametrized against Large and Chemically Diverse Training Sets: Are They More Accurate and/or Robust than Double-Hybrid DFT?" *Journal of Chemical Theory and Computation* **2020**, 16, 4238–4255.

(5) **Semidalas, E. C.**; Semidalas, C. E., "Structure and Vibrational Spectra of p-Coumaric Acid Dimers by DFT Methods" *Vibrational Spectroscopy* **2019**, 101, 100–108.

(4) **Semidalas, E.** C.; Semidalas, C. E., "Argo: A Data Analysis Program for Quantum Chemical Calculations" *Journal of Molecular Modeling* **2019**, 25, 82.

(3) **Semidalas, E.**; Chrissanthopoulos, A., "Computational Study of Structural, Vibrational and Electronic Properties of the Highly Symmetric Molecules M_4S_6 (M = P, As, Sb, Bi)" *Computational and Theoretical Chemistry* **2019**, 1149, 41–48.

(2) Zarkadoulas, A.; Koutsouri, E.; **Semidalas, E.**; Psycharis, V.; Raptopoulou, C. P.; Mitsopoulou, C. A., "Photocatalytic Hydrogen Production with Alkylated Nickel Bis-Dithiolene Complexes" *Polyhedron* **2018**, 152, 138–146.

(1) Semidalas, C.; **Semidalas, E.**; Matsoukas, M. T.; Nixarlidis, C.; Zoumpoulakis, P., "In Silico Studies Reveal the Mechanisms behind the Antioxidant and Anti-Inflammatory Activities of Hydroxytyrosol" *Medicinal Chemistry Research*

2016, 25, 2498–2511.

Publications in Conference Proceedings

(3) **Semidalas, E.**; Santra, G.; Mehta, N.; Martin, J. M. L., "S66 Noncovalent Interactions Benchmark Re-Examined: Composite Localized Coupled Cluster Approaches" *AIP Conference Proceedings* **2022**, 2611, 020016.

(2) Martin, J. M. L.; Santra, G.; **Semidalas, E**., "An Exchange-Based Diagnostic for Static Correlation" *AIP Conference Proceedings* **2022**, 2611, 020014.

(1) **Semidalas, E.**; Viras, K.; Chatzigeorgiou P.; Kellici T.; Leonis G.; Mavromoustakos T.; Semidalas, E., "The Effects of Vinblastine in the Lipid Bilayers" *SCinTe*, **2015**, 3, 176.

Book Chapter

Leonis, G.; **Semidalas, E. C.**; Chatzigeorgiou, P.; Pollatos, E.; Semidalas, C. E.; Rappolt, M.; Viras, K.; Mavromoustakos, T., "Vinblastine. In *Advances in Biomembranes and Lipid Self-Assembly"*, **2019**, 29, 127–157.

Book Translation

Μοριακή κβαντική μηχανική, **Semidalas E.**, Papazissi Publications, 2023, Greek translation and scientific editing of Molecular quantum mechanics, Peter Atkins and Ronald Friedman, 5th edition, Oxford University Press, **2011**.

Lectures at Scientific Conferences

8/11/2021-11/11/2021 **Semidalas, E.**; Santra, G.; Mehta, N.; Martin, J. M. L., "S66 Revisited: Composite Localized Coupled Cluster Approaches" CECAM Flagship Workshop: Benchmarking of Electronic Structure Methods for Non-Covalent Interactions (online participation) **2021**, Paris, France

5/11/2015–7/11/2015 **Semidalas, E.**; Viras K.; Chatzigeorgiou P.; Kellici T.; Leonis G.; Mavromoustakos T.; Semidalas C., "The Effects of Vinblastine in the Lipid Bilayers" *SCinTE* **2015**, Athens, Greece

Posters at Scientific Conferences

12/9/2022 Santra, G.; **Semidalas E.**; Martin, J. M. L., "Remarkable Performance of XYG3 Family Functionals Using a Scaled GLPT3 Correlation" 86th Israeli Chemical Society Annual Meeting, **2022**, Tel Aviv, Israel

3/7/2022–8/7/22 **Semidalas, E.**; Martin, J. M. L., "The MOBH35 Metal-Organic Barrier Heights Reconsidered: Performance of Local-Orbital Coupled Cluster Approaches in Different Static Correlation Regimes" 12th Triennial Congress of the World Association of Theoretical and Computational Chemists **2020**, Vancouver, Canada

Contributions to the Scientific Community/Public Activities/Military Service

- Reviewer for Theoretical Chemistry Accounts, Springer
- Member of the Israeli Chemical Society
- Interview in the Greek newspaper Kathimerini on: 'Excellence is rewarded in Israel', February 13, 2019, www.kathimerini.gr/society/1009783/sto-israil-i-aristeia-epivraveyetai/

- Military service from 3/2018 until 12/2018 at the Hellenic Force of Cyprus (ELDYK), Nicosia, Cyprus