CV of Stefan Vučković

Website: www.stefanvuckovic.com

Date and place of birth: 1 June 1990, Belgrade (Serbia); Nationality: Dutch (NL), Serbian (RS)

Current Employment

- From April 2023: Assistant Professor and Theoretical Chemistry Group Leader at Department of Chemistry, University of Fribourg, Av. de l'Europe 20, CH-1700 Fribourg, Switzerland

Previous Employment

- 2021-2023 Marie Sklodowska-Curie fellow at the CNR Italy, CNR-IMM institute Lecce, Italy
- 2021- Humboldt postdoctoral fellow at the University of Saarland University, Germany
- 2018 – 2021 Rubicon Postdoctoral Fellow in the group of Kieron Burke at the University of California, Irvine

Education

PhD: **Nov. 2013 – Nov. 2017:** VU University Amsterdam with **cum laude distinction (highest distinction awarded to PhDs in the Netherlands and it is received by less than 10% of candidates)** Supervisor: Prof. Dr. Paola Gori-Giorgi;

B.S in Chemistry **Oct. 2009- Jun 2013*:*** Faculty of Chemistry, University in Belgrade, Serbia; **Best Student of the class and of University in Belgrade.**

Major Funding

ERC Starting Grant: **1.5M EUR** 2025-2030
SNSF Starting Grant **1.8M EUR:** 2023- 2028
SNSF Ambizione Grant: **900k EUR** *(respectfully declined)*
University Research Fellowships by UK's Royal Society **830k £** *(respectfully declined)*
Marie Skłodowska-Curie Individual Fellowships by REA, **170k EUR** 2021-2023
Germany Humboldt Foundation Research Fellowship for Postdoctoral Researchers **100k EUR** 2021
Rubicon postdoc awarded by NWO (Netherlands Organisation or Scientific Research), **170k EUR** 2018-2020
Newton international postdoc fellowship awarded by the UK's Royal Society, **100 k £** ***(****respectfully declined)*

Invited Talks

1. CECAM "Accelerating Improvements in Density Functional Theory", August 2023, Lausanne, Switzerland
2. 2023 TDDFT School & Workshop: Excited states and dynamics, July 2023, Newark, USA
3. International Congress on Molecular Electronic Structures, September 2022, Tunisia
4. Oxford Theory Seminar, University of Oxford, October 2021, UK
5. European Theoretical Spectroscopy Facility (ETSF) seminar, April 2021, France
6. Max Planck Society Group Leader Symposium, February 2021, Germany
7. Molecular Electronic Structure Conference, September 2020, Warsaw, Poland
8. HRSMC Annual Symposium 2018*, November 2018*, Leiden, Netherlands
9. DFT and optimal transport with Coulomb cost workshop, August 2015, Amsterdam, Netherlands

Contributed Talks

1. American Chemical Society (ACS) Fall meeting, March 2022, Chicago, USA
2. 60th Sanibel Meeting: "The Theory Meeting for Theoreticians", February 2020, St. Simons Is., Georgia, hot-topic session
3. 18th International Conference on Density Functional Theory and its Applications, July 2019, Alicante, Spain

4. American Chemical Society (ACS) Fall meeting, August 2017, Washington DC, USA
5. DPG Annual meeting, March 2017, Dresden, Germany
6. American Physical Society March Meeting, March 2016, Baltimore, USA
7. CHAINS - Dutch Chemistry Conference, December 2015, Veldhoven, Netherlands
8. 12th ETSF Young Researchers' Meeting: Challenges in ab initio modelling of materials, June 2015, Paris, France
9. CHAINS 2014, Dutch Chemistry Conference, December 2014, Veldhoven, Netherlands

Awards/Prices

2022: 2022 Electronic Structure emerging leader focus issue invitation
2020: Löwdin Outstanding Postdoc award, Sanibel symposium 2020
2019: Computation 2019 Travel Award 2k EUR
2018 The Dick Stufkens Prize 2018 for the best PhD thesis of the Holland Research School of Molecular Chemistry (HRSMC) 2k EUR
2017 Travel award ACS Fall meeting 2017 600$
2013-2017 Talent support for Serbian PhD students abroad 30k EUR 2013 Best BS student a the University in Belgrade (Serbia) award

Demonstrated Independence

- My research independence is most clearly evidenced by the three single-author and other publications without my PhD advisor (Paola Gori Giorgi) and my postdoc advisor (Kieron Burke). As can be seen from the "Major Funding" section above, ever since I completed my PhD I have obtained the funding for my project and was the PI in my projects.
- For the period of six months, I have been leading my Theoretical Chemistry group at Chemistry Department University of Fribourg (Switzerland) and during this period I have: **(1)** published three papers as lead author; **(2)** gave two invited talks; **(3)** received two major grants (see the "Major Funding" section above); **(4)** received an invitation to be a gest editor for two collections of the Machine Learning Science and Technology journal.

Publications

h-index: 16 (see Google Scholar page: https://scholar.google.com/citations?user=VXoB2VQAAAAJ&hl=sr)

27. Gould, T.; Chan, B.; Dale, S. G.; **Vuckovic, S*.** Transferable diversity – a data-driven representation of chemical space. 10.26434/chemrxiv-2023-5075x-v2.
26. Daas, K. J.; Kooi, D. P.; Peters, N. C.; Fabiano, E.; Della Sala, F.; Gori-Giorgi, P.; **Vuckovic, S*.** Regularized and Opposite Spin-Scaled Functionals from Møller–Plesset Adiabatic Connection─Higher Accuracy at Lower Cost. J. Phys. Chem. Lett. 2023, 14, 8448.
25. **Vuckovic, S*.**; Bahmann, H. Nonlocal Functionals Inspired by the Strongly Interacting Limit of DFT: Exact Constraints and Implementation. J. Chem. Theory Comput. 2023, 19, 6172.
24. **Vuckovic, S*.** Using AI to Navigate through the DFA Zoo. Nat Comput Sci 2023, 3, 6. Sole-author work
23. Song, S.; **Vuckovic, S.**; Kim, Y.; Yu, H.; Sim, E*.; Burke, K. Extending Density Functional Theory with near Chemical Accuracy beyond Pure Water. Nat Commun 2023, 14, 799. Featured article.
22. **Vuckovic, S*.**; Gerolin, A.; Daas, T. J.; Bahmann, H.; Friesecke, G.; Gori-Giorgi, P*. Density functionals based on the mathematical structure of the strong-interaction limit of DFT. WIREs Comput Mol Sci 2022, 13.
21. **Vuckovic, S*.** Quantification of Geometric Errors Made Simple: Application to Main-Group Molecular Structures. J. Phys. Chem. A 2022, 126, 1300. Sole-author work
20. Sim, E*.; Song, S.; **Vuckovic, S.**; Burke, K. Improving Results by Improving Densities: Density-Corrected Density Functional Theory. J. Am. Chem. Soc. 2022, 144, 6625.
19. Song, S.; **Vuckovic, S.**; Sim, E. *; Burke, K. Density-Corrected DFT Explained: Questions and Answers. J. Chem. Theory Comput. 2022, 18, 817.
18. Daas, T. J.; Fabiano, E.; Della Sala, F.; Gori-Giorgi, P.; **Vuckovic, S.** Noncovalent Interactions from Models for the Møller-Plesset Adiabatic Connection. J. Phys. Chem. Lett. 2021, 12, 4867.
17. Song, S.; **Vuckovic, S.**; Sim, E. *; Burke, K. Density Sensitivity of Empirical Functionals. J. Phys. Chem. Lett. 2021, 12, 800.

16. Gerrits, N.; Smeets, E. W. F.; **Vuckovic, S.**; Powell, A. D.; Doblhoff-Dier, K.; Kroes, G.-J*****. Density Functional Theory for Molecule–Metal Surface Reactions: When Does the Generalized Gradient Approximation Get It Right, and What to Do If It Does Not. J. Phys. Chem. Lett. 2020, 11, 10552.
15. **Vuckovic, S.**; Burke, K*****. Quantifying and Understanding Errors in Molecular Geometries. J. Phys. Chem. Lett. 2020, 11, 9957.
14. Daas, T. J.; Grossi, J.; **Vuckovic, S.**; Musslimani, Z. H.; Kooi, D. P.; Seidl, M.; Giesbertz, K. J. H.; Gori-Giorgi, P.***** Large Coupling-Strength Expansion of the Møller–Plesset Adiabatic Connection: From Paradigmatic Cases to Variational Expressions for the Leading Terms. The Journal of Chemical Physics 2020, 153, 214112.
13. **Vuckovic, S. ***; Fabiano, E.; Gori-Giorgi, P.; Burke, K. MAP: An MP2 Accuracy Predictor for Weak Interactions from Adiabatic Connection Theory. J. Chem. Theory Comput. 2020, 16, 4141.
12. **Vuckovic, S.**; Song, S.; Kozlowski, J.; Sim, E.; Burke, K.***** Density Functional Analysis: The Theory of Density-Corrected DFT. J. Chem. Theory Comput. 2019, 15, 6636.
11. Gould, T.; **Vuckovic, S.*** Range-Separation and the Multiple Radii Functional Approximation Inspired by the Strongly Interacting Limit of Density Functional Theory. The Journal of Chemical Physics 2019, 151, 184101. Editor's Pick.
10. **Vuckovic, S. *** Density Functionals from the Multiple-Radii Approach: Analysis and Recovery of the Kinetic Correlation Energy. J. Chem. Theory Comput. 2019, 15, 3580.
9. Seidl, M.; Giarrusso, S.; **Vuckovic, S**.; Fabiano, E.; Gori-Giorgi, P.***** Communication: Strong-Interaction Limit of an Adiabatic Connection in Hartree-Fock Theory. The Journal of Chemical Physics 2018, 149, 241101.
8. Giarrusso, S.; **Vuckovic, S.;** Gori-Giorgi, P.***** Response Potential in the Strong-Interaction Limit of Density Functional Theory: Analysis and Comparison with the Coupling-Constant Average. J. Chem. Theory Comput. 2018, 14, 4151.
7. **Vuckovic, S.***; Gori-Giorgi, P.; Della Sala, F.; Fabiano, E. Restoring Size Consistency of Approximate Functionals Constructed from the Adiabatic Connection. J. Phys. Chem. Lett. 2018, 9, 3137.
6. **Vuckovic, S.***; Levy, M.; Gori-Giorgi, P. Augmented Potential, Energy Densities, and Virial Relations in the Weak- and Strong-Interaction Limits of DFT. The Journal of Chemical Physics 2017, 147, 214107. JCP Editors' Choice 2017.
5. **Vuckovic, S.***; Gori-Giorgi, P. Simple Fully Nonlocal Density Functionals for Electronic Repulsion Energy. J. Phys. Chem. Lett. 2017, 8, 2799. Highlighted by ACS in Spotlights.
4. **Vuckovic, S.*;** Irons, T. J. P.; Wagner, L. O.; Teale, A. M.; Gori-Giorgi, P. Interpolated Energy Densities, Correlation Indicators and Lower Bounds from Approximations to the Strong Coupling Limit of DFT. Phys. Chem. Chem. Phys. 2017, 19, 6169.
3. **Vuckovic, S.;** Irons, T. J. P.; Savin, A.; Teale, A. M.; Gori-Giorgi, P.***** Exchange–Correlation Functionals via Local Interpolation along the Adiabatic Connection. J. Chem. Theory Comput. 2016, 12, 2598. ACS Editors' choice.
2. Seidl, M.; **Vuckovic, S.;** Gori-Giorgi, P.***** Challenging the Lieb–Oxford Bound in a Systematic Way. Molecular Physics 2016, 114, 1076.
1. **Vuckovic, S.;** Wagner, L. O.; Mirtschink, A.; Gori-Giorgi, P.***** Hydrogen Molecule Dissociation Curve with Functionals Based on the Strictly Correlated Regime. J. Chem. Theory Comput. 2015, 11, 3153.