Dr Stephanie C. C. van der Lubbe

Designations:
Research Fellow / Data Scientist, Division of Family Medicine, Yong Loo Lin School of Medicine, National University of Singapore (NUS)
Research Fellow, Department of Family Medicine, National University Health System (NUHS)

Qualifications:
PhD (Vrije Universiteit Amsterdam, Netherlands)
MSc (Vrije Universiteit Amsterdam, Netherlands)

Dr. Stephanie is a research fellow and data scientist at the Division of Family Medicine (NUS). She obtained her Masters in Chemistry (Molecular Simulation and Photonics) in 2016, and obtained her PhD in computational chemistry with cum laude distinction. After working one more year in Amsterdam as a postdoctoral fellow, Stephanie started as a research fellow in the Department of Materials Science and Engineering at the National University of Singapore. In this position, she applied computational models on next-generation batteries and worked on model development and data analysis using Python. In April 2023, she started as a research fellow and data scientist in the division of Family Medicine.

Research Interests

- Data analytics
- Artificial intelligence in primary care
- Chronic disease management
- Primary cancer care

Journals & Publications

1. VV Lee, SCC van der Lubbe, LH Goh, JM Valderas, Harnessing ChatGPT for thematic analysis: Are we ready? arXiv:2310.14545 (**2023**).
2. SCC van der Lubbe, P Canepa, Modeling the Effects of Salt Concentration on Aqueous and Organic Electrolytes, *npj Comput. Mater.* **2023**, 175.
3. SCC van der Lubbe, Z Wang, DKJ Lee, P Canepa, Unlocking the Inaccessible Energy Density of Sodium Vanadium Fluorophosphate Electrode Materials by Transition Metal Mixing, *Chem. Mater.* **2023**, *35*, 5116.
4. D Almacellas, SCC van der Lubbe, AA Grosch, I Tsagri, P Vermeeren, J Poater, C Fonseca Guerra, Non-Innocent π Linkers Affect Cooperativity in Hydrogen-Bonded Macrocycles, *ChemistryEurope* **2023**, e202300036.
5. L de Azevedo Santos, D Cesario, P Vermeeren, SCC van der Lubbe, F Nunzi, C Fonseca Guerra, σ-Electrons Responsible for Cooperativity and Ring Equalization in

Hydrogen-Bonded Supramolecular Polymers, *ChemPlusChem* **2022**, *87*, e202100436 (Cover and cover profile).

6. F Zaccaria, SCC van der Lubbe, C Nieuwland, TA Hamlin, C Fonseca Guerra, How Divalent Cations Interact with the Internal Channel Site of Guanine Quadruplexes, *ChemPhysChem* **2021**, *22*, 2265 (Cover and cover profile)
7. L de Azevedo Santos, SCC van der Lubbe, TA Hamlin, TC Ramalho, FM Bickelhaupt, A Quantitative MO Perspective of the Chalcogen Bond, *ChemistryOpen* **2021**, *10*, 391 (Cover and cover profile).
8. SCC van der Lubbe, A Haim, T van Heesch, C Fonseca Guerra, Tuning the binding strength of even and uneven hydrogen-bonded arrays with remote substituents, *J. Phys. Chem A* **2020**, *124*, 9451 (Cover).
9. SCC van der Lubbe, P Vermeeren, C Fonseca Guerra, FM Bickelhaupt, The Nature of Nonclassical Carbonyl Ligands Explained by Kohn-Sham Molecular Orbital Theory, *Chem. Eur. J.* **2020**, *26*, 15690 (Issue #1000).
10. J Chen, J Wang, SCC van der Lubbe, M Cheng, D Qiu, D Monchaud, J Mergny, C Fonseca Guerra, H Ju, J Zhou, A push-pull mechanism helps designing highly competent G-quadruplex-DNA catalysts, *CCS Chem.* **2020**, *2*, 2183.
11. E Margiotta, SCC van der Lubbe, L de Azevedo Santos, G Paragi, S Moro, FM Bickelhaupt, C Fonseca Guerra, Halogen Bonds in Ligand-Protein Systems: Molecular Orbital Theory for Drug Design, *J. Chem. Inf. Model.* **2020**, *60*, 1317.
12. P Vermeeren, SCC van der Lubbe, C Fonseca Guerra, FM Bickelhaupt, TA Hamlin, Understanding Chemical Reactivity Using the Activation Strain Model, *Nat. Protoc.* **2020**, *15*, 649.
13. SCC van der Lubbe, C Fonseca Guerra, The Nature of Hydrogen Bonds: A Delineation of the Role of Different Energy Components on Hydrogen Bond Strengths and Lengths, *Chem. Asian J.* **2019**, *14*, 2760 (Cover).
14. SCC van der Lubbe, F Zaccaria, X Sun, C Fonseca Guerra, Secondary Electrostatic Interaction Model Revised: Prediction Comes Mainly from Measuring Charge Accumulation in Hydrogen-Bonded Monomers, *J. Am. Chem. Soc.* **2019**, *141*, 4878 (Cover).
15. HM Coubrough, SCC van der Lubbe, K Hetherington, A Minard, C Pask, MJ Howard, C Fonseca Guerra, AJ Wilson, Supramolecular Self-Sorting Networks Using Hydrogen-Bonded Motifs, *Chem. Eur. J.* **2019**, *25*, 785 (Cover).
16. A Grosch, SCC van der Lubbe, C Fonseca Guerra, Nature of Intramolecular Resonance Assisted Hydrogen Bonding in Malonaldehyde and Its Saturated Analogue, *J. Phys. Chem. A* **2018**, *122*, 1813.
17. SCC van der Lubbe, C Fonseca Guerra, Hydrogen Bond Strength of CC and GG Pairs Determined by Steric Repulsion: Electrostatics and Charge Transfer Overruled, *Chem. Eur. J.* **2017**, *23*, 10249 (Hot paper, cover and cover profile).

Updated 27 Nov 2023