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Start Time: Wednesday, February 8, 2023 05:15 pm

End Time: Wednesday, February 8, 2023 06:30 pm

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and via Zoom

Data-driven chemical understanding with geometrical and quantum-chemical bonding analysis

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Chemical bonding and coordination environments are crucial descriptors of material properties. They have previously been applied to creating chemical design guidelines and chemical heuristics.[1] They are currently being used as features in machine learning more and more frequently.[2] I will discuss implementations and algorithms (ChemEnv and LobsterEnv) for identifying these coordination environments based on geometrical characteristics and chemical bond quantum chemical analysis.[3–5] I will demonstrate how these techniques helped in testing chemical heuristics like the Pauling rule and thereby improved our understanding of chemistry.[6] I will also show how these tools can be used to create new design guidelines and a new understanding of chemistry.[4,7] To use quantum-chemical bonding analysis on a large-scale and for machine-learning approaches, fully automatic workflows and analysis tools have been developed.[4,8] After presenting the capabilities of these tools, I will also point out how these developments relate to the general trend towards automation in the field of density functional based materials science.[9]

References

[1] J. George, G. Hautier, Trends in Chemistry 2021, 3, 86–95.

[2] A. M. Ganose, A. Jain, MRS Commun. 2019, 9, 874–881. [3] D. Waroquiers, J. George, M. Horton, S. Schenk, K. A. Persson, G.-M. Rignanese, X. Gonze, G. Hautier, Acta Cryst B 2020, 76, 683–695.

[4] J. George, G. Petretto, A. Naik, M. Esters, A. J. Jackson, R. Nelson, R. Dronskowski, G.-M. Rignanese, G. Hautier, ChemPlusChem 2022, e202200123, DOI: 10.1002/cplu.202200123.

[5] R. Nelson, C. Ertural, J. George, V. L. Deringer, G. Hautier, R. Dronskowski, J. Comput. Chem 2020, 41, 1931–1940.

[6] J. George, D. Waroquiers, D. Di Stefano, G. Petretto, G. Rignanese, G. Hautier, Angew. Chem. Int. Ed. 2020, 59, 7569–7575.

[7] W. Chen, J. George, J. B. Varley, G.-M. Rignanese, G. Hautier, Npj Comput. Mater. 2019, 5, 72.

[8] “LobsterPy,” can be found under github.com/JaGeo/LobsterPy, 2022.

[9] J. George, Trends Chem. 2021, 3, 697–699.

Dr. Ariane Feirrera Nunes Alves

Organizer