

UniSysCat - Colloquium

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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

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- [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.
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- [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 Feirrer Nunes Alves

Organizer