A Quantitative Molecular Orbital Perspective of the Chalcogen Bond

Invited for this month’s cover are the groups of Prof. Dr. Teodorico C. Ramalho (Federal University of Lavras and University Hradec Královo) and Prof. Dr. F. Matthias Bickelhaupt (Vrije Universiteit Amsterdam and Radboud University). The cover picture shows the key message of their work, that is, the covalency of the chalcogen bonds, in an elegantly simple and attractive manner. To that end, the chalcogen bonds are represented by schematic 3D structures of the bond donor D_{2}Ch and the bond acceptor A⁻, and their attractive interaction in green. Then, a colorful molecular orbital (MO) diagram where the HOMO–LUMO mixing is represented by the mixing of red (HOMO) and blue (LUMO) into purple (MO) is presented. Read the full text of their Full Paper at 10.1002/open.202000323.

What is the most significant result of this study?
We exhibit the covalent character of the chalcogen bonds through sound and quantitative analyses and highlight their similarities with other well-known intermolecular interactions, such as halogen-, and hydrogen bonds. These findings counter the (oversimplified) view that chalcogen bonds are purely or predominantly electrostatic. We hope these insights provide experimentalists and theoreticians with a unified framework to rationalize chalcogen bonds and similar interactions.

Who designed the cover?
The cover was designed by Lucas de Azevedo Santos and Dr. Trevor A. Hamlin. Special thanks to members of the TheoCheM group for their critical and insightful suggestions.

What was the inspiration for this cover design?
We sought to highlight the key message of our work, that is, the covalency of the chalcogen bonds, in an elegantly simple and attractive manner. To that end, the chalcogen bonds are represented by schematic 3D structures of the bond donor D_{2}Ch and the bond acceptor A⁻, and their attractive interaction in green. Then, a colorful molecular orbital (MO) diagram where the HOMO–LUMO mixing is represented by the mixing of red (HOMO) and blue (LUMO) into purple (MO) is presented.
These concepts are further reinforced (albeit subconsciously) by a colorful background that depicts the mixing of colors, akin to the mixing of orbitals and corresponding flow of electron density.

What aspects of this project do you find most exciting?
It is always exciting to have the chance to perform a ‘deep dive’ into a topic of fundamental research. Equipped with the right tools, one can discover answers for phenomena occurring at atomic level that may never be fully explained by experiments. Modern computational chemistry methods are accurate enough to allow theoreticians to challenge established concepts or fill the gaps of incomplete pictures. This is exactly what we did for chalcogen bonds in this contribution to *ChemistryOpen*.