Electron density, and its interplay with the energy and properties of molecules and solids

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Electron density has been a great source of insight in the understanding of bonding and structure. Nonetheless, it lacks a fundamental characteristic: its connection to molecular and solid properties is barely predictive. This is so due to the lack of a direct (known) link between electron density and energetics.
Along this contribution we will try to show some of the efforts of my team to fill this gap. My first example will be the characterization of non-covalent interactions in reactivity. In order to build this knowledge, we rely on the **Non Covalent Interactions (NCI) index**, which is able to identify the regions relevant to weak interactions from the electron density alone [1]. Simple approaches for well-known intermolecular energies datasets have allowed us to show that the energy can be predicted from these electron density regions using machine learning approaches in a fast and accurate manner [2]. I will also show a new server, NCIweb, we have developed to carry out these calculations online [3].

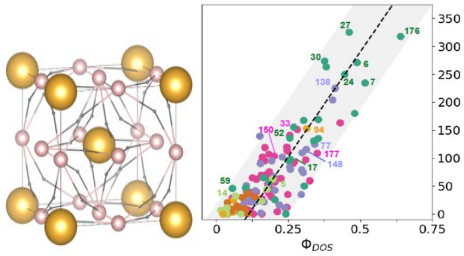

Figure 1. Example of delocalization pathways in H3S (left) and networking correlation with superconductors critical temperatures (right).

Secondly, I will show an example of prediction of material properties such as **superconductivity**. We have shown that the networking value, derived from chemical bonding analysis, correlates well with the predicted critical temperature, much better than any other descriptor analyzed thus far. And this, for all bonding types [4].

The discovery of the positive correlation between superconductivity and the bonding network offers the possibility of screening easily hydrogen-based compounds and, at the same time, sets clear paths for chemically engineering better superconductors.

References

1. E. R. Johnson, S. Keinan, P. Mori-Sanchez, J. Contreras-Garcia, A. J. Cohen, and W. Yang, "Revealing Noncovalent Interactions", J. Am. Chem. Soc. 132, 6498 (2010).
2. F. Peccati, E. Desmedt, J. Contreras-Garcia* "A Regression Approach to Accurate Interaction Energies Using Topological Descriptors Computational and Theoretical Chemistry", Comp. Theo. Chem., 1159, 23 (2019).
3. T. Novoa, R. Laplaza, F. Peccati, F. Fuster, J. Contreras-Garcia*, "The NCIWEB Server: A Novel Implementation of the Noncovalent Interactions Index for Biomolecular Systems", J. Chem. Inf. Model. 63, 15 (2023).
4. F. Belli, T. Novoa, J. Contreras-Garcia, I. Errea, "Strong correlation between electronic bonding network and critical temperature in hydrogen-based superconductors", Nature Communications 12, 5381 (2021).

CURRICULUM VITAE

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Julia Contreras is Directrice de Recherche au CNRS, leading the CHemical Interpretation team at Laboratoire de Chimie Théorique (LCT, UMR7616). One of her main areas of research is non covalent interactions (with over 5000 citations). She also wrote the code to visualize this index, NCIPLOT. The associated paper was published in 2011 in JCTC and it has received over 2600 citations and more than 13000 visits. She is chair of the European Committee of High Pressure and president of the FWO chemistry panel. Most recently her interests have turned into superconductivity, where we have been able for the first time to introduce an index that describes superconductivity from fast calculations (Nature Communications 12, 5381 (2021)). During these years she has given 43 invited talks and published more than 100 articles. She has also been involved in the creation of scientific associations (European Committee of Chemical Bonding, Women Under High Pressure).