Chemical Concepts from a Momentum-Space Perspective

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The far majority of chemists almost uniquely use the position representation of quantum mechanics in their study of atoms and molecules. This is due to the familiarity of this representation and its direct link to molecular structures, including conformations, chirality etc. and many so-called chemical concepts.

Some authors have, over the years, tried to recover chemical concepts in momentum space through a plethora of ways such as studying momentum density plots[1], attempts at defining atoms in molecules from a momentum perspective[2] or have used the momentum space valence bias to use in studying the similarity of molecules[3]. A relative newcomer is the study of Domain Averaged Fermi Holes (DAFH) in momentum space.

This lecture highlights the merits of many of these approaches but also shows how e.g., previous atoms in molecules methods apparently seem to work by "a lucky mathematical problem". DAFH may sometimes reveal more subtle bonding phenomena but implicitly rely on some position space steps in between[4] whereas even for diatomics, provided a large data set, fingerprinting chemical bonds in momentum space seems rather difficult.

Finally, attention will be devoted to testing how good the latest density functionals perform for momentum space densities.

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[3] Allan, N.L.; D.L. Cooper, *Top. Curr. Chem.*, **1995**, *173*, 85.

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