Self-Attractive Hartree Decomposition: Partitioning Electron Density into Smooth Localized Fragments - DTU Orbit (18/01/2019)

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Chemical bonding plays a central role in the description and understanding of chemistry. Many methods have been proposed to extract information about bonding from quantum chemical calculations, majority of them resorting to molecular orbitals as basic descriptors. Here, we present a method called Self-Attractive Hartree (SAH) decomposition, to unravel pairs of electrons directly from electron density, which unlike molecular orbitals, is a well defined observable that can be accessed experimentally. The key idea is to partition the density into a sum of one-electron fragments which simultaneously maximize self-repulsion and maintain regular shapes. This leads to a set of rather unusual equations, in which every electron experiences self-attractive Hartree potential in addition to an external potential common for all the electrons. The resulting symmetry breaking and localization are surprisingly consistent with chemical intuition. SAH decomposition is also shown to be effective in visualization of single/multiple bonds, lone pairs and unusual bonds due to the smooth nature of fragment densities. Furthermore, we demonstrate that it can be used to identify specific chemical bonds in molecular complexes and provides a simple and accurate electrostatic model of hydrogen bonding.

General information
State: Accepted/In press
Organisations: Massachusetts Institute of Technology
Contributors: Zhu, T., de Silva, P., Voorhis, T. V.
Number of pages: 37
Publication date: 2017
Peer-reviewed: Yes

Publication information
Journal: Journal of Chemical Theory and Computation
ISSN (Print): 1549-9618
Ratings:
BFI (2019): BFI-level 2
Web of Science (2019): Indexed yes
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 5.25 SJR 2.497 SNIP 1.476
Web of Science (2017): Impact factor 5.399
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.37 SJR 2.711 SNIP 1.51
Web of Science (2016): Impact factor 5.245
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 5.65 SJR 2.702 SNIP 1.643
Web of Science (2015): Impact factor 5.301
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 5.63 SJR 2.803 SNIP 1.588
Web of Science (2014): Impact factor 5.498
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 5.41 SJR 2.437 SNIP 1.569
Web of Science (2013): Impact factor 5.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 5.34 SJR 2.784 SNIP 1.614
Web of Science (2012): Impact factor 5.389
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2