

Anatomy of Bond Formation. Insights from the Analysis of Domain-Averaged Fermi Holes in Momentum Space

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Alongside conventional domain-averaged Fermi hole (DAFH) analysis in position space, we examine an alternative representation in momentum space. As examples we consider the processes of splitting the chemical bonds in the simple diatomic molecules H_2 , N_2 and LiH , as representatives of non-polar single, non-polar multiple, and polar bonding. We believe that the additional information provided by the complementary description in momentum space contributes to a better understanding of the phenomenon of chemical bonding.

Key words: momentum space; domain-averaged Fermi holes; bond formation