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Momentum Densities

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Abstract:

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Scalar fields are useful for gaining knowledge of the features of any chemical system. Electron momentum density (EMD) is a scalar field, which brings out chemical concepts from the momentum-space point of view. The topography of EMD has been extensively studied and analyzed. One important characteristic of the molecular EMDs is the bond-directionality principle, which states that the maximal nature of the EMD is perpendicular to the position space bonding directions. This allows us to relate, interpret and understand phenomena such as bonding and ionization via molecular properties in the momentum space. This

may bear applications for, and better understanding of laser-induced bond-forming and bond-breaking in molecules.

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