Holographic Principles of Molecular Structure and Electron Density Calculations

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Electron densities of molecules obey a holographic principle: in a non-degenerate ground state any small positive volume of the electron density cloud contains the complete information about the entire molecular structure [1]. This holographic theorem provides the constraint on the applications of various electron density fragmentation methods, including fuzzy density fragmentation methods aimed at potential advances in the crystallographic structure refinement process [2], the analysis of quantum chemical functional groups of molecules [3], detailed molecular shape analysis [4], and providing the foundations for linear scaling, ab inito quality macromolecular quantum chemistry computational methods, applied to various proteins [5-7]. Some new advances in these fields will be reviewed.

[1] Mezey P.G., *Mol. Phys.,* 1999, **96**, 169. [2] Mezey P.G., *Adv. Molec. Structure Res.,* 1998, **4**, 115. [3] Mezey P.G., *Adv. Quant. Chem.,* 1996, **27**, 163. [4] Mezey P.G., *Shape in Chemistry: an Introduction to Molecular Shape and Topology,* VCH, New York, 1993. [5] Mezey P.G., *Int. J. Quant. Chem.,* 1997, **63**, 39. [6] Mezey P.G., *Pharmaceutical News,* 1997, **4**, 29. [7] Exner T.E., Mezey P.G., *J. Comput. Chem.,* 2003, **24**, 1980.

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