A Viewpoint on Population Analyses

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Abstract

Population analyses have become an indispensable tool to computational chemists. Yet implementation within popular quantum chemistry software has buried the interesting philosophical choices made when partitioning the electron density into atomic contributions. There is further historical context that has significantly influenced common conceptions of chemical bonding and reactivity. This work reviews select aspects of orbital and spatial decomposition schemes of the density matrix, pointing out essential linear algebraic considerations and associated tools of shared interest to us and Prof. Mayer.

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