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A Look at the Quantum Theory of Atoms in Molecules from the Discrete Morse Theory

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Abstract : The quantum theory of atoms in molecules (QTAIM) allows us to obtain topological information on electronic density in quantum mechanical systems. The QTAIM starts by considering the electron density as a continuous mathematical object. On the other hand, the discretization of electron density is also a mathematical object, which, from discrete mathematics, would allow a new approach to its topological study. From this point of view, it is necessary to develop a series of steps that provide the theoretical support that guarantees its application. Some of the steps that we consider most important are mentioned below: (1) obtain good representations of the electron density through computational calculations, (2) design a methodology for the discretization of electron density, and construct the simplicial complex. (3) Make an analysis of the discrete vector field associating the simplicial complex. (4) Finally, in this research, we propose to use the discrete Morse theory as a mathematical tool to carry out studies of electron density topology.

Keywords : discrete mathematics, Discrete Morse theory, electronic density, computational calculations
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