On the topology of the reduced density gradient

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Non-covalent interactions (NCIs) play a key role in many areas of science, ranging from biochemistry to condensed matter. In this regard, the NCI index, as a new tool to identify and characterize weak interaction of various strengths as chemical intuitive reduced density gradient (RDG) isosurfaces that reveal both stabilizing (hydrogen-bonding and van der Waals interactions) and destabilizing interactions.[1] Beyond qualitative analysis, the integration of both volume and charge within NCI isosurfaces are in good agreement with the hydrogen-bonding potential-energy surfaces. [2] Recently Saleh *et al.* found a good linear correlation between stabilization energies and kinetic energies integrated on the main NCI isosurfaces. [3] These results connect the topology of the reduced density gradient with energetics.

In this work we present the latest version of the NCIPLOT code: NCIPLOT 4.0. This version is capable of performing topological analysis of the reduced density gradient isosurfaces: localization of critical points, computation of flux lines and integration of different quantum mechanical properties. As a proof of principle we apply our code to the analysis to characterize non-covalent interaction in a self-assembly monolayer (SAM) system such as octylamine/platinum. [4]

Reference

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