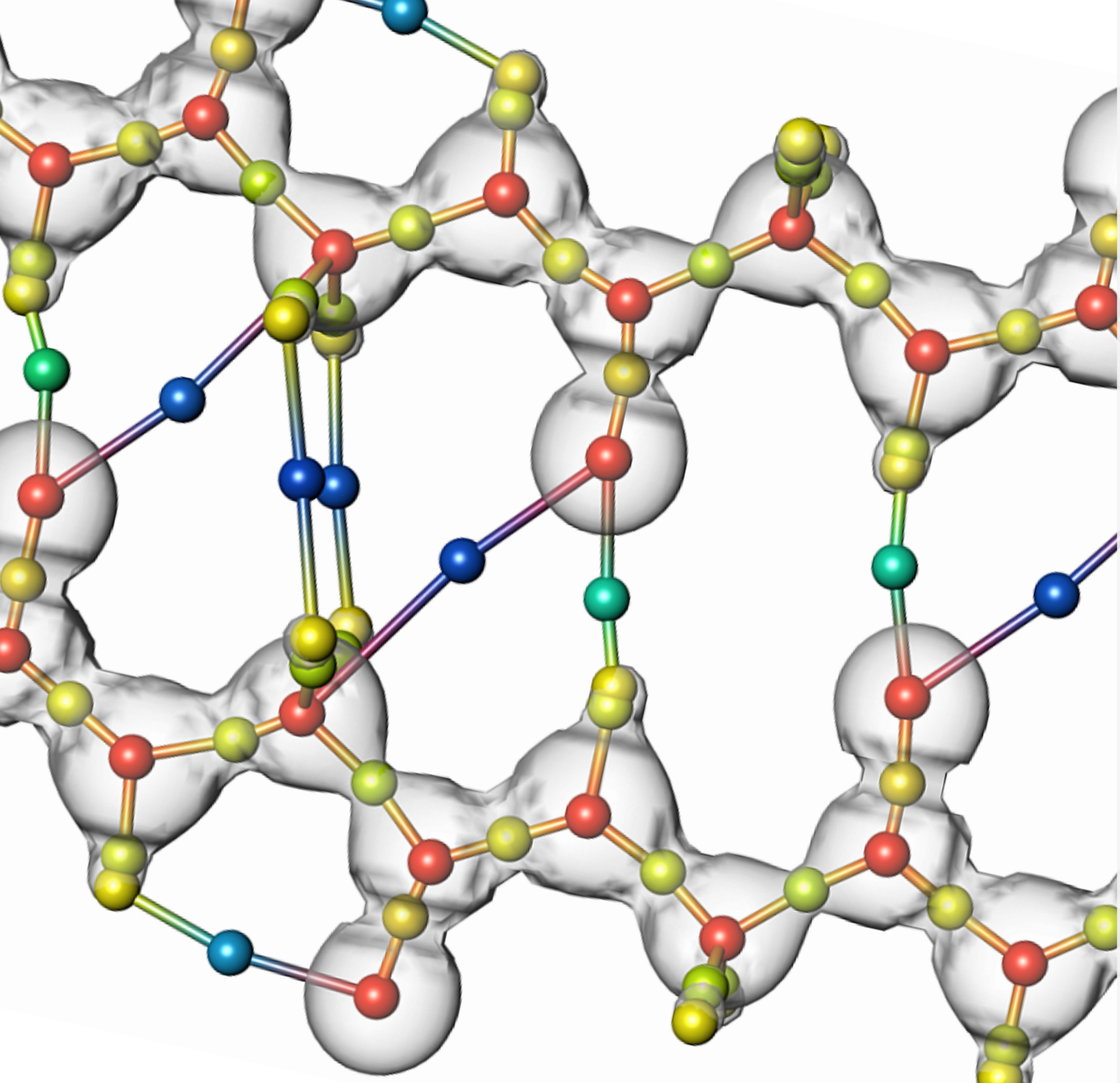

Characterizing Molecular Interactions in Chemical Systems

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Interactions between atoms have a major influence on the chemical properties of molecular systems. While covalent interactions impose the structural integrity of molecules, noncovalent interactions govern more subtle phenomena such as protein folding, bonding or self assembly. The understanding of these types of interactions is necessary for the interpretation of many biological processes and chemical design tasks. While traditionally the electron density is analyzed to interpret the quantum chemistry of a molecular system, noncovalent interactions are characterized by low electron densities and only slight variations of them – challenging their extraction and characterization. Recently, the signed electron density and the reduced gradient, two scalar fields derived from the electron density, have drawn much attention in quantum chemistry since they enable a qualitative visualization of these interactions even in complex molecular systems and experimental measurements.

In this work, we present the first combinatorial algorithm for the automated extraction and characterization of covalent and noncovalent interactions in molecular systems. The proposed algorithm is based on a joint topological analysis of the signed electron density and the reduced gradient. Combining the connectivity information of the critical points of these two scalar fields enables to visualize, enumerate, classify and investigate molecular interactions in a robust manner. Experiments on a variety of molecular systems, from simple dimers to proteins or DNA, demonstrate the ability of our technique to robustly extract these interactions and to reveal their structural relations to the atoms and bonds forming the molecules. For simple systems, our analysis corroborates the observations made by the chemists while it provides new visual and quantitative insights on chemical interactions for larger molecular systems.

Paper