Structure and regularity of molecular eigenfunctions and electron densities

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We study the structure of the eigenfunctions of the Hamilton-operator for a molecule near the singularities of the potential. By a product-'Ansatz', we characterize the singularities of the eigenfunctions up to class $C^{1,1}$. The obtained information is applied to study the structure and regularity of the corresponding electron density. In particular, we prove that the density is smooth away from the nuclei. This is joint work with S. Fournais, M. and T. Hoffmann-Ostenhof.