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The Nature of the Metal-Metal Multiple Bond

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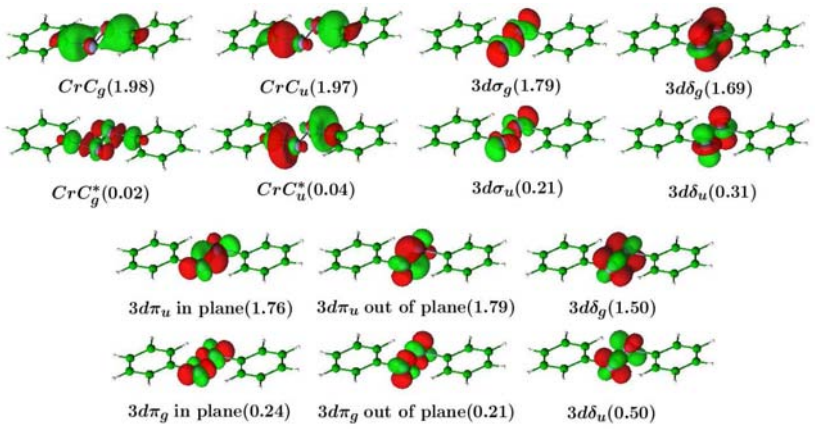
The chemical bond between the heavier elements in the periodic table is more complex than those between light atoms and the theoretical description becomes more complicated. There are mainly two reasons for this increased complexity. One is relativity. Starting with the first row transition metals, relativistic effects starts to play a role for the chemical behavior of the compounds. This effect increases considerably for the second and third row, where it is a dominant feature. This is also true for heavy main group elements and for lanthanides and actinides. The second reason is the increased complexity of the electronic structure of the atoms, the high density of states, and the sometimes weak chemical bonds. This leads to complicated electronic structures that are not easily described with standard quantum chemical tools. I will in this lecture show some features of chemical bonding for some illustrative examples, including metal-metal multiple bonding and the chemical bonds in actinides. These results have been obtained using a multiconfigurational quantum chemical method and I shall also give a brief overview of the general features of this approach and explain why it is suitable to study heavy element chemistry.



The molecules orbitals of the chemical bond between the two chromium atoms in the compounds PhCrCrPh.