Bonding Pattern Change Induced by Relativistic Effects

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The periodic table provides a fundamental protocol for qualitatively classifying and predicting chemical properties based on periodicity. While the periodic law of chemical elements had already been rationalized within the framework of the nonrelativistic description of chemistry with quantum mechanics, this law was later known to be affected significantly by relativity. Here we report that relativistic effects change the bond multiplicity of the group 6 diatomic molecules M_2 (M = Cr, Mo, W, Sg) from hextuple bonds for Cr_2, Mo_2, W_2 to quadruple bond for Sg_2, thus breaking the periodicity in the nonrelativistic domain. Besides, we here also report a systematic theoretical study on the chemical bonding pattern change in the coinage metal dimers (Cu_2, Ag_2, Au_2, Rg_2) due to the relativistic effect on the superheavy elements. Unlike the lighter congeners basically demonstrating ns−ns bonding character ground state, Rg_2 shows unique 6d−6d bonding induced by strong relativity.

References

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