Basis set superposition error in atomic cluster calculations

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In this work, the basis set superposition error (BSSE) has been analyzed for the systems Cu2, Cu3, Cu6 and Cu13 as prototypes of metallic clusters. Various basis sets have been tested. In addition, pseudopotentials of 1- and 19-valence electrons have also been studied in relationship to the BSSE. The results are conclusive. At the present, it is almost impossible to do an all-electron calculation in transition-metal clusters without great error in basis set superposition, even for clusters of moderate size. The only solution seems to be using pseudopotentials with a carefully chosen basis set.