PSEUDOPOTENTIALS FOR SUPERHEAVY ELEMENTS

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Energy adjusted pseudopotentials for the elements with 111 to 118 protons (Eka-Gold to Eka-Radon) are described. The generation method is briefly outlined followed by a discussion of some issues that are more important for superheavy elements than for the lighter elements. These issues include: the choice of data for a spin-averaged pseudopotential, the derivation of the spin-orbit part of a pseudopotential and the use of separate basis sets for non-relativistic, scalar relativistic and spin-orbit calculations. Some test calculations where the pseudopotential results are compared with all-electron data along with a quick outline of other calculations where these pseudopotentials have been used are also given.