THEORETICAL STUDY OF LOW-LYING STATES OF UH

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Large-scale multireference configuration-interaction (MRCI) calculations using the all-electron scalar-relativistic Douglas-Kroll-Hess (DKH) Hamiltonian, as well as a relativistic energy-consistent small-core pseudopotential (SPP) for uranium, have been performed to study the low-lying electronic ΛS states of uranium monohydride UH with term energies below 0.5 eV. After taking spin-orbit effects into account both DKH/MRCI and SPP/MRCI calculations predict a $^4I_{9/2}$ ground state. The calculated ground state molecular constants of both approaches show a good agreement with each other (MRCI+Q, DKH: Re=2.021 Å, ω_e=1483 cm^{-1}, D_e=2.79 eV; SPP: R_e=2.011 Å, ω_e=1497 cm^{-1}, D_e=2.85 eV), as well as with available experimental data (ω_e=1424 cm^{-1} in argon matrix).