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A quantum Monte Carlo study of thorium halide molecules SHI GUO, MINYI ZHU, North Carolina State University, ENRIQUE BATISTA, RICHARD MARTIN, Los Alamos National Lab, LUBOS MITAS, North Carolina State University — We present electronic structure calculations of thorium halide molecules, namely, a series of $ThCl_n$ and $ThBr_n$ (n=1,2,3,4) systems. We calculate the bond dissociation energies for the sequence of the following dissociation reactions: $ThCl_n -> ThCl_{n-1} + Cl$ and $ThBr_n -> ThBr_{n-1} + Br$. We apply both large core and small core energy-consistent pseudopotentials for thorium atom and we employ DFT GGA and hybrid functionals for energies and geometry calculations. For high accuracy energies we use the fixed-node diffusion Monte Carlo (DMC) method. In DMC calculations we employ both single- and multi-reference trial wave functions in order to test the quality of the nodal surfaces. We study the dissociation energies with regard to different multiplicities of the ThX_n molecules and the different behavior of the bromides with respect to chlorides. We compare our results with hybrid DFT methods and experimental values. Supported by DOE and NSF.

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