EXTENDING ACCURATE QUANTUM CHEMISTRY TO HEAVY ELEMENTS

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The presentation will be focused on development and applications of relativistic wave function-based approaches aiming to extend the accuracy and applicability of quantum chemistry to heavy elements. An atomic mean-field spin-orbit approach within exact two-component theory, the X2CAMF scheme, is shown to enhance the computational efficiency while retaining the accuracy of the parent four-component Dirac-Coulomb-Breit approach. An efficient implementation of the X2CAMF scheme together with analytic energy gradients for spin-orbit coupled-cluster methods enables accurate calculations of geometries and properties for molecules containing heavy atoms. The applicability of these relativistic quantum-chemical methods is demonstrated with applications in heavy-element chemistry and spectroscopy.