Computational Methodologies for Molecules and Materials Containing *f* Electrons

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Understanding the chemistry of rare-earth and actinide elements is essential for addressing challenges in nuclear energy, critical materials, and nuclear waste management. Our research integrates theoretical and computational chemistry to investigate the electronic structure, bonding, and chemical behavior of *f*-element systems. By combining quantum chemical method development with applications in rare-earth and actinide chemistry, we investigate how relativistic effects, electron correlation, and chemical environment influence molecular properties and spectroscopic behavior. Current research areas include relativistic electronic structure theory, rare-earth element separations, and actinide chemistry. Through collaborations with experimental researchers, we seek to connect fundamental electronic structure with observable chemical phenomena.