APPLICATION OF RELATIVISTIC DENSITY FUNCTIONAL THEORY TO THE STRUCTURE AND BONDING OF ACTINIDE AND TRANSACTINIDE MOLECULAR SYSTEMS

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The use of relativistic density functional theory calculations to address the structure and bonding in molecular systems of the actinide and transactinide elements will be presented. The chemical systems to be discussed will include organoactinide sandwich compounds, An(η^n-$C_nH_n)_2$, hydrated actinide ions, and explorations into transactinide main-group chemistry.