

High Performance, High precision Multiresolution Calculation of Core-Level Shifts

T. D. Engeness and T. A. Arias

Multiresolution analysis (MRA) of electronic structure affords the opportunity to capture the full physics of the atomic cores in a systematically improvable manner. Applying new techniques, we demonstrate for the first time that MRA of all-electron calculations can be carried out to high precision with the same computational effort as the corresponding pseudopotential calculation, which neither captures the full core physics nor is systematically improvable. With this approach, we present calculations of paramagnetic core-level shifts where local density-functional theory is the sole approximation.