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Electronic Structure Calculations for Heavy Elements: Radon (Z=86) and Francium (Z=87) ALEXANDER KOUFOS, DIMITRIOS PAPACONSTANTOPOULOS, George Mason University — Electronic structure calculations allow scientists to predict the properties of solids without the use of physical material. Although the ability to manipulate matter has improved dramatically within the past couple decades, some matter is still hard to study. Modern computers not only let us study this matter, but allow us to do it more quickly and just as accurately. The electronic structure of two rare and mostly unstudied elements, Radon (Z=86) and Francium (Z=87), has been calculated. The augmented plane wave (APW) method with local density approximation (LDA) functional as well as the linearized augmented plane wave (LAPW) method with both LDA and generalized gradient approximation (GGA) functionals were used to perform the calculations. Francium total energy calculations gave the fcc structure slightly below the bcc structure with a minimal energy difference of $\Delta E = 0.33mRy$. The difference found is consistent with other alkali metal total energy calculations which do not verify the bcc structure to be the ground state. Radon was predicted to be an insulator with a gap of $0.931Ry$ similar to the other noble gases.

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