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## **(G\*) Atomic Shell Structure of the Entire Periodic Table Using an Alternative Approach to Orbital-Free Density-Functional Theory**

*Wednesday, 8 June 2022 13:15 (15 minutes)*

The principal aim of orbital-free density-functional theory (OF-DFT) over its competitors is to reduce the computational effort required to efficiently calculate properties of quantum systems, thereby increasing the feasibility of many applications to large interacting systems. A novel implementation of OF-DFT is achieved using the isomorphism between classical statistical mechanics in 3+1 dimensions and quantum statistical mechanics in 3 dimensions, to which quantum density-functional theory is replaced with polymer self-consistent field theory for ring polymers. This new OF-DFT is used to calculate the electron densities and their associated binding energies for every element on the periodic table, using a simple Fermi-Amaldi exchange-correlation potential and an Edwards-Flory-Huggins interaction potential from polymer physics to represent the Pauli exclusion effect. The theory predicts quantitatively accurate electron densities (where sufficient experimental data exist for comparison) and binding energies within 5% of the experimentally measured values for elements up to Cadmium, drifting beyond this mark for heavier elements due to the increasing importance of relativistic effects in these atoms.

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