Canadian Association of Physicists
Association canadienne des physiciens et physiciennes

Contribution ID: **3056** Type: **Oral Competition (Graduate Student) / Compétition orale (Étudiant(e) du 2e ou 3e cycle)**

(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.

Authors: LEMAITRE, Phil; THOMPSON, Russell (University of Waterloo)

Presenter: LEMAITRE, Phil

Session Classification: W2-10 DAMOPC I (DAMOPC) | DPAMPC I (DPAMPC)

Track Classification: Technical Sessions / Sessions techniques: Atomic, Molecular and Optical Physics, Canada / Physique atomique, moléculaire et photonique, Canada (DAMOPC-DPAMPC)