



Canadian Association
of Physicists

Association canadienne
des physiciens et physiciennes

Contribution ID: 163 Type: **Poster Competition (Graduate Student) / Compétition affiches (Étudiant(e) 2e ou 3e cycle)**

(G*) POS-H79 – Homonuclear diatomic molecule properties from an orbital-free-related density functional theory

Wednesday 9 June 2021 14:03 (2 minutes)

An orbital free related density functional theory based on the principles of polymer self-consistent field theory is used to calculate the electron densities, bond energy, bond length and fundamental vibrational frequency of homonuclear diatomic molecules. A simple exchange-correlation functional that neglects correlations is used, and the Pauli potential is based on Edwards–Flory-Huggins interaction taken from polymer physics. Other approximations include a Fermi-Amaldi correction for electron-electron self-interactions and cylindrical averaging to reduce the dimensionality of the problem. Expected bonding characteristics are observed for the first 7 elements in the periodic table. Specifically, quantitatively accurate bond lengths and qualitatively accurate bond energy structure for hydrogen and nitrogen molecules. Bond energy and fundamental vibrational frequency are discrepant up to a factor of two when compared with accepted values. Other elements do not exhibit bonding as expected.

Authors: SILLASTE, Spencer (University of Waterloo); Prof. THOMPSON, Russell (University of Waterloo)

Presenter: SILLASTE, Spencer (University of Waterloo)

Session Classification: W-POS-H #75-79,109 Poster session (DTP) / Session d'affiches (DPT)

Track Classification: Theoretical Physics / Physique théorique (DTP-DPT)