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

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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.

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