Understanding Atoms and Covalent Bonds - An Exploration by Thomas-Fermi and One-Electron Theories

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Abstract

Within this thesis we revisit important fields in physical chemistry as atoms, molecules and their covalent bonds with the aim of making these topics easier to understand for students and nonexpert colleagues. The research developments have in the past been intended almost exclusively to advance the knowledge of experts. Little emphasis has been placed on developing theory for the express purpose of making a fact or a phenomenon easy to understand. Within this work we therefore place a great deal of emphasis on just this aspect. We would like to derive and present simplified theories which make it as easy as possible for students and nonexpert colleagues to acquire expert knowledge in important areas. Thus we start from existing important knowledge obtained by rather complex theories and ask whether there are simpler theories which can better explain and serve as a pedagogical stepping stone on the way to expert knowledge.

The important knowledge and related theories which we revisit in this work are related to atomic structure, atomic reactivity and covalent bonding. The simplified theories are derived from Thomas-Fermi theory which is a semiclassical density functional theory. The Thomas-Fermi theory is not as accurate as the modern Hartree-Fock theory or density functional theory but it is much simpler and can nevertheless describe some of the main features of these theories.

These simplified theories are then implemented into texts and visual computational tools which have been included into a physical chemistry textbook written in Swedish. The textbook is used in the second year of chemistry at Göteborg University. The visual computational tools are evaluated in the course.

Keywords: quantum ergodicity, delocalization, covalent bonding, atomic reactivity, Thomas - Fermi theory.