An Explicit Approach to Conceptual Density Functional Theory Descriptors of Arbitrary Order

Farnaz Heidar-Zadeh, Michael Richer, Stijn Fias, Ramón Alain Miranda-Quintana, Matthew Chan, Marco Franco-Pérez, Cristina E. González-Espinoza, Taewon David Kim, Caitlin Lanssens, Anand H.G. Patel, Xiaotian Derrick Yang, Esteban Vöhringer-Martínez, Carlos Cárdenas, Toon Verstraelen, Paul W. Ayers

PII: S0009-2614(16)30528-0
DOI: http://dx.doi.org/10.1016/j.cplett.2016.07.039
Reference: CPLETT 34033

To appear in: *Chemical Physics Letters*

Received Date: 22 May 2016
Accepted Date: 18 July 2016

Please cite this article as: F. Heidar-Zadeh, M. Richer, S. Fias, R.A. Miranda-Quintana, M. Chan, M. Franco-Pérez, C.E. González-Espinoza, T.D. Kim, C. Lanssens, A.H.G. Patel, X.D. Yang, E. Vöhringer-Martínez, C. Cárdenas, T. Verstraelen, P.W. Ayers, An Explicit Approach to Conceptual Density Functional Theory Descriptors of Arbitrary Order, *Chemical Physics Letters* (2016), doi: http://dx.doi.org/10.1016/j.cplett.2016.07.039

An Explicit Approach to Conceptual Density Functional Theory Descriptors of Arbitrary Order

Farnaz Heidar-Zadeh[a,b,c], Michael Richer[a], Stijn Fias[d], Ramón Alain Miranda-Quintana[a,e], Matthew Chan[a,b,c], Marco Franco-Pérez[a], Cristina E. González-Espinoza[a], Taewon David Kim[a], Caitlin Lanssens[a,b], Anand H. G. Patel,[a] Xiaotian Derrick Yang[a], Esteban Vöhringer-Martínez[f], Carlos Cárdenas,[g,h] Toon Verstraelen[c], and Paul W. Ayers[*a]

Abstract:

We present explicit formulas for arbitrary-order derivatives of the energy, grand potential, electron density, and higher-order response functions with respect to the number of electrons, and the chemical potential for any smooth and differentiable model of the energy versus the number of electrons. The resulting expressions for global reactivity descriptors (hyperhardnesses and hypersoftnesses), local reactivity descriptors (hyperFukui functions and local hypersoftnesses), and nonlocal response functions are easy to evaluate computationally. Specifically, the explicit formulas for global/local/nonlocal hypersoftnesses of arbitrary order are derived using Bell polynomials. Explicit expressions for global and local hypersoftness indicators up to fifth order are presented.

a. Department of Chemistry & Chemical Biology; McMaster University; Hamilton, Ontario, Canada

b. Department of Inorganic and Physical Chemistry, Ghent University, Krijgslaan 281 (S3), 9000 Gent, Belgium

c. Center for Molecular Modeling, Ghent University, Technologiepark 903, 9052 Zwijnaarde, Belgium

d. General Chemistry (ALGC), Vrije Universiteit Brussel, Pleinlaan 2, 1050 Brussel, Belgium

e. Laboratory of Computational and Theoretical Chemistry, Faculty of Chemistry, University of Havana, Havana, Cuba

f. Departamento de Físico-Química, Facultad de Ciencias Químicas, Universidad de Concepción, Concepción, Chile

g. Departamento de Física, Facultad de Ciencias, Universidad de Chile.

h. Centro para el Desarrollo de la Nanociencia y la Nanotecnología (CEDENNA), Avda. Ecuador 3493, Santiago 9170124, Chile.

[*] ayers@mcmaster.ca