Delocalization error of density-functional approximations: A distinct manifestation in hydrogen molecular chains

By: Zheng, X (Zheng, Xiao)[1,2] ; Liu, M (Liu, Min)[2] ; Johnson, ER (Johnson, Erin R.)[3] ; Contreras-Garcia, J (Contreras-Garcia, Julia)[4] ; Yang, WT (Yang, Weitao)[5,6]

View ResearcherID and ORCID

JOURNAL OF CHEMICAL PHYSICS
Volume: 137 Issue: 21
Article Number: 214106
DOI: 10.1063/1.4768673
Published: DEC 7 2012
View Journal Impact

Abstract

Delocalization error is one of the major sources of inaccuracy for mainstream density functional approximations and it is responsible for many of the most glaring failures. Quantitative identification of delocalization error in chemical species and analysis of its influence on calculated thermodynamic properties have remained scarce. In this work we demonstrate unambiguously the effect of delocalization error on a series of hydrogen molecular chains and elucidate the underlying relationship between the error magnitude and system geometry. This work stresses the necessity of minimizing delocalization error associated with density functional approximations. (C) 2012 American Institute of Physics. [http://dx.doi.org/10.1063/1.4768673]

Keywords

KeyWords Plus: FRACTIONAL PARTICLE NUMBER; ELECTRON LOCALIZATION; DERIVATIVE DISCONTINUITIES; TOPOLOGICAL ANALYSIS; DFT FUNCTIONALS; ENERGY; EXCHANGE; SYSTEMS; OLIGOMERS; BONDS

Author Information

Reprint Address: Zheng, X (reprint author)

+ Univ Sci & Technol China, Hefei Natl Lab Phys Sci Microscale, Hefei 230026, Anhui, Peoples R China.

Addresses:

+ [1] Univ Sci & Technol China, Hefei Natl Lab Phys Sci Microscale, Hefei 230026, Anhui, Peoples R China

+ [2] Univ Sci & Technol China, Dept Chem Phys, Hefei 230026, Anhui, Peoples R China

+ [3] Univ Calif Merced, Dept Chem & Chem Biol, Merced, CA 95343 USA

[4] Lab Chim Theor, F-75005 Paris, France

+ [5] Duke Univ, Dept Chem, Durham, NC 27708 USA

− [6] King Abdulaziz Univ, Fac Sci, Jeddah 21589, Saudi Arabia
Organization-Enhanced Name(s)
King Abdulaziz University

E-mail Addresses: xz58@ustc.edu.cn; ejohnson29@ucmerced.edu; weitao.yang@duke.edu

Funding

Funding Agency	Grant Number
NSF of China	21103157 21233007
Fundamental Research Funds for the Central Universities	2340000034 2340000025
Office of Naval Research	N00014-09-1-0576
National Science Foundation	CHE-09-11119
Spanish Ministry of Education	Orden EDU/22532010

View funding text

Publisher

AMER INST PHYSICS, CIRCULATION & FULFILLMENT DIV, 2 HUNTINGTON QUADRANGLE, STE 1 N O 1, MELVILLE, NY 11747-4501 USA

Categories / Classification

Research Areas: Chemistry; Physics

Web of Science Categories: Chemistry, Physical; Physics, Atomic, Molecular & Chemical

Document Information

Document Type: Article

Language: English

Accession Number: WOS:000312252900006

PubMed ID: 23231216

ISSN: 0021-9606

eISSN: 1089-7690

Other Information

IDS Number: 053EH

Cited References in Web of Science Core Collection: 41

Times Cited in Web of Science Core Collection: 17