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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]

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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]

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