Accepted Manuscript

Title: Gauging the performance of some density functionals including dispersion and nonlocal corrections for relative energies of water 20-mers

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PII: \$1093-3263(17)30282-6

DOI: http://dx.doi.org/doi:10.1016/j.jmgm.2017.05.006

Reference: JMG 6915

To appear in: Journal of Molecular Graphics and Modelling

Received date: 16-4-2017 Revised date: 10-5-2017 Accepted date: 11-5-2017

Please cite this article as: Mojtaba Alipour, Gauging the performance of some density functionals including dispersion and nonlocal corrections for relative energies of water 20-mers, Journal of Molecular Graphics and Modellinghttp://dx.doi.org/10.1016/j.jmgm.2017.05.006

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ACCEPTED MANUSCRIPT

Gauging the performance of some density functionals including dispersion and nonlocal corrections for relative energies of water 20-mers

Mojtaba Alipour *

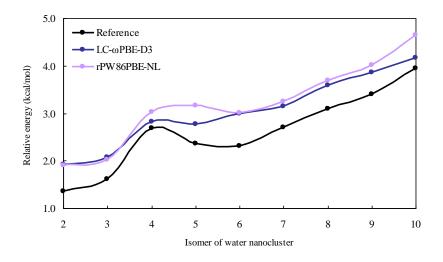
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Graphical Abstract



Highlights:

- Relative energies of the isomers of (H₂O)₂₀ nanocluster have been predicted.
- Dispersion and nonlocal corrections of DFT have been assessed.

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