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**Influence of Molecular Size on the Density-Functional Delocalization Error** SARAH WHITTLETON, ALBERTO OTERO-DE-LA-ROZA, ERIN JOHNSON, University of California, Merced — While density-functional theory (DFT) is an effective and popular method in quantum chemistry and physics, approximations within the exchange-correlation functional can produce substantial inaccuracies. For example the local density approximation (LDA) and generalized-gradient approximation (GGA) produce convex energy versus charge curves that violate the correct piecewise-linearity constraint of  $E(N)$  for fractional charges, referred to as delocalization error. This leads to a false description of molecular properties, such as the HOMO and LUMO energy levels. This work investigates the delocalization error in a series of gas-phase organic molecules including alkanes, alkenes, alkynes, allenes, and polycyclic aromatic hydrocarbons. The GGA deviation from linearity of the  $E(N)$  curves is evaluated and  $\omega$ -tuning of a long-range corrected functional is performed for each molecule. It is found that the deviation from linearity and thus the optimal  $\omega$ , decrease with increasing molecular size. However, systematic error in the endpoint of the  $E(N)$  curve, and thus in the ionization potential, is simultaneously introduced, demonstrating the impact of molecular size on delocalization error.

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