Abstract Submitted
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Testing and using the Lewin-Lieb bounds in density functional theory[1] DAVID FEINBLUM, Department of Chemistry, University of California, Irvine, JOHN KENISON, Department of Physics and Astronomy, University of California, Irvine, KIERON BURKE, Department of Chemistry, University of California, Irvine — Lewin and Lieb have recently proven several new bounds on the exchange-correlation energy that complement the Lieb-Oxford bound. We test these bounds for atoms, for slowly-varying gases, and for Hooke's atom, finding them usually less strict than the Lieb-Oxford bound. However, we also show that, if a generalized gradient approximation (GGA) is to guarantee satisfaction of the new bounds for all densities, new restrictions on the the exchange-correlation enhancement factor are implied.

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