Testing and using the Lewin-Lieb bounds in density functional theory\textsuperscript{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 exchange-correlation enhancement factor are implied.

\textsuperscript{1}We thank Mathieu Lewin and Elliott Lieb for bringing their new bounds to our attention, and Eberhard Engel for developing the OPMKS atom code. This work was supported by NSF under grant CHE-1112442.