Nuclear Fukui functions from nonintegral electron number calculations

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Numerical results for the nuclear Fukui function (NFF) based on a nonintegral number of electrons methodology (NIEM) are reported for a series of simple diatomic molecules. A comparison with those obtained from other methodologies is focused on the estimation of the error associated with a finite difference approximation for the evaluation of the NFF. The dependence of NFFs on the type and size of the basis set is also discussed. The NIEM values are in close agreement with those obtained from a finite difference approximation using ?N = ±1 with large basis sets.