Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary material to "DFT-based genetic algorithm search for AuCu nanoalloy electrocatalysts for CO_2 reduction"

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Included in this supplementary material is plots for correcting the LCAO adsorption energies for COOH, CHO and OH against values calculated with the plane wave code DACAPO. As opposed to the CO correction in the main paper, where all LCAO energies were underestimated, we here find errors to both sides. Thus an extra error value is reported here; the mean of the absolute errors (MAE) as well as the average error (AvgE) and the standard deviation (stdev).

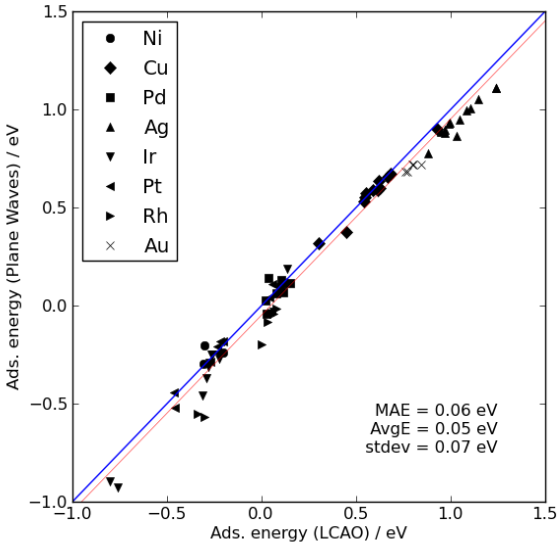

Figure S1: Adsorption energies of COOH with the plane wave code DACAPO vs. LCAO mode in GPAW

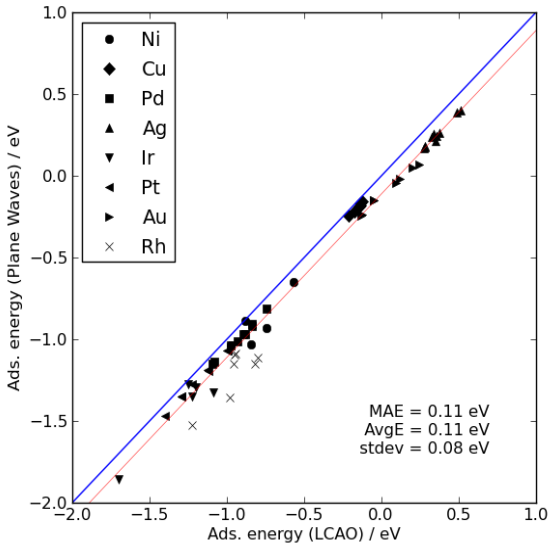

Figure S2: Adsorption energies of CHO with the plane wave code DACAPO vs. LCAO mode in GPAW

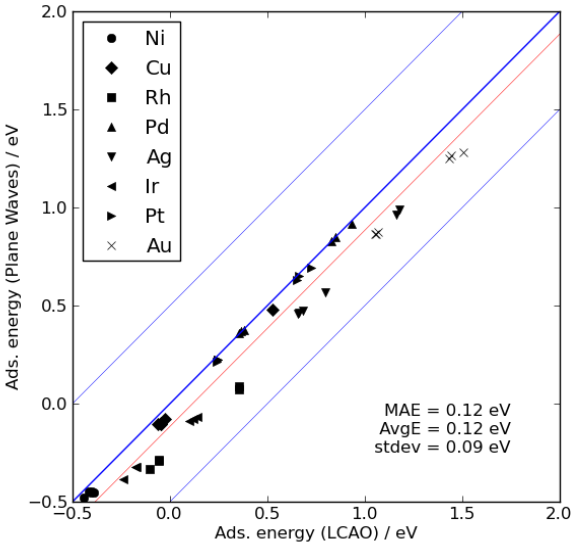

Figure S3: Adsorption energies of OH with the plane wave code DACAPO vs. LCAO mode in GPAW