Addendum to “Convergence of density and hybrid functional defect calculations for compound semiconductors”

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This paper reported first-principles supercell calculations for the formation enthalpy ΔH of numerous charged defects in several semiconductors and insulators. The individual energy contributions leading to the final result for ΔH , as given in Table IV of the original paper, were not included in the original submission. This Addendum provides detailed data allowing the interested reader to retrace the steps that lead to the final result, accessible through the Supplemental Material [1].

[1] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/PhysRevB.96.239903> for the atomic structures (primitive and supercells) and for a spreadsheet containing the individual energy contributions leading to the final results in ΔH .