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Correction

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Correction to Understanding the Optimal Adsorption Energies for Catalyst Screening in Heterogeneous Catalysis

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Two papers by Kozuch and Shaik (A Combined Kinetic−Quantum Mechanical Model for Assessment of Catalytic Cycles: Application to Cross-Coupling and Heck Reactions, *J. Am. Chem. Soc.*, **2006**, *128*, 3355−3365 and Kinetic-Quantum Chemical Model for Catalytic Cycles: The Haber-Bosch Process and the Effect of Reagent Concentration, *J. Phys. Chem. A*, **2008**, *112*, 6032−6041)[1,2] on energetic span theory were mistakenly not cited in the published letter[3] due to an error in the editing of the final manuscript, and we apologize for this oversight. We fully recognize the significant contributions that the papers of Kozuch and Shaik have made to the field and the relevance to the published ACS catalysis paper. In particular, in ref 2, the authors proposed two equations from the framework of the energy span theory for the optimal adsorption energy, which are similar to eqs 10 and 11 derived in our work.

REFERENCES

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(2) Kozuch, S.; Shaik, S. *J. Phys. Chem. A* **2008**, *112*, 6032−6041.
(3) Yang, B.; Burch, R.; Hardacre, C.; Headdock, G.; Hu, P. *ACS Catal.* **2014**, *4*, 182−186.

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