Supporting Information

Correction to “C-H Bond Activation of Light Alkanes on Pt(111): Dissociative Sticking Coefficients, Evans-Polanyi Relation, and Gas-Surface Energy Transfer”

[*J. Phys. Chem. C* 2010, **114**, 17222, DOI: 10.1021/jp105073g]

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Revised Figure Captions

Figure 2. Methane dissociative sticking coefficients on Pt(111) for the impinging gas temperatures indicated. The solid points (expts) and lines (simulations) are for normally directed effusive molecular beams. The open points (expts) and dashed lines (simulations) are for ambient gas impingement. The PC-MURT simulations are based on a parameter set, $\{E_0 = 56 \text{ kJ/mol}, s = 3, \nu_D = 125 \text{ cm}^{-1}\}$,³ that reproduces a wide variety of methane/Pt(111) supersonic molecular beam experiments.^{5,8}

Figure 3. Methane dissociative sticking coefficients on Pt(111) are compared with (a) PC-MURT simulations based on the parameter set, $\{E_0 = 48.2 \text{ kJ/mol}, s = 4, \nu_D = 315 \text{ cm}^{-1}\}$, and (b) Master Equation (ME)-MURT simulations that additionally incorporate gas-surface energy transfer with exponential down parameter $\alpha = 50 \text{ cm}^{-1}$.

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Figure 4. Ethane dissociative sticking coefficients on Pt(111) are compared with (a) PC-MURT simulations based on the parameter set, $\{E_0 = 34.4 \text{ kJ/mol}, s = 4, \nu_D = 145 \text{ cm}^{-1}\}$, and (b) ME-MURT simulations that additionally incorporate gas-surface energy transfer with exponential down parameter $\alpha = 700 \text{ cm}^{-1}$.

Figure 5. Propane dissociative sticking coefficients on Pt(111) are compared with (a) PC-MURT simulations based on the parameter set, $\{E_0 = 21.2 \text{ kJ/mol}, s = 4, \nu_D = 70 \text{ cm}^{-1}\}$, and (b) ME-MURT simulations that additionally incorporate gas-surface energy transfer with exponential down parameter $\alpha = 1400 \text{ cm}^{-1}$. The directed effusive beam sticking coefficients for which $T_g = T_s$ are additionally labeled by encirclement.

Figure 6. Arrhenius plot of quasi-thermal dissociative sticking coefficients, $S_n(T)$, for several alkanes on Pt(111) with one standard deviation error bars included. The effusive molecular beam was incident along the direction of the surface normal with $T_g = T_s = T$. Table 2 lists the parameters of the fitted Arrhenius lines.

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Supplementary Information: Revised Figures

Figure 2

Figure 3

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Figure 5

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