Supporting Information for

Interfacial and Alloying Effects on Activation of Ethanol from First Principles

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Table S1. Calculated lattice constant and surface segregation energy (Seg. E) of Rh in Rh_1M_3 alloy

Bulk	Cal. (Å)	Exp. (Å)	Seg. E (eV/Rh atom)*
Rh	3.844	3.804	–
Ir	3.881	3.839	-0.04
Ru**	2.731,4.307	2.7058,4.2816	-0.45
Pd	3.951	3.891	0.33
Cu	3.632	3.615	0.08
Au	4.171	4.078	0.59

*Negative (positive) segregation energy denotes preference of forming surface alloy (near surface alloy). Data retrieved from ref.[1]

**Hexagonal-close packed (hcp) metal.

References

(1) Ruban, A. V.; Skriver, H. L.; Norskov, J. K., Surface Segregation Energies in Transition-Metal Alloys. *Phys. Rev. B* **1999**, *59*, 15990-16000.