Supplementary Information

How Coverage Influences Thermodynamic and Kinetic Isotope Effects for H_2/D_2 Dissociative Adsorption on Transition Metals

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S1. Convolution of Thermodynamic and Kinetic Isotope Effects

Thermodynamic and kinetic isotope effects (TIEs and KIEs) of individual elementary steps are convoluted in the observed experimental KIEs for the overall reaction. Consider the following simple reaction mechanism for the hydrogenation of species A with 3 elementary steps E1–E3:

$$\mathrm{A(g)} + * \rightleftharpoons \mathrm{A}\,, \tag{E1}$$

$$\mathrm{H_2(g)} + 2* \rightleftharpoons 2\mathrm{H}, \tag{E2}$$

$$\mathrm{A} + \mathrm{H} \rightarrow \mathrm{AH(g)} + 2*, \tag{E3}$$

where * denotes a vacant site.

If E3 is the rate determining step, then the overall rate of reaction is:

$$\mathrm{r} = \mathrm{k_3}\theta_\mathrm{H}\theta_\mathrm{A,} \tag{S1}$$

where θ_H and θ_A are the coverages of H and A respectively, and $\mathrm{k_3}$ is the rate constant of elementary step 3.

Assuming elementary steps 1 and 2 are quasi-equilibrated, the coverages of H, A, and vacant sites are:

$$\theta_H = \sqrt{K_2 P_{H_2}}\,\theta_* \tag{S2}$$

$$\theta_A = K_1 P_A \theta_* \tag{S3}$$

$$\theta_* = 1 - \theta_A - \theta_H = \frac{1}{1 + K_1 P_A + \sqrt{K_2 P_{H_2}}}, \tag{S4}$$

where K_1 and K_2 are the equilibrium constants for elementary steps 1 and 2 respectively, θ_* is the coverage of vacant sites, and P_A and P_{H_2} are the partial pressures of A(g) and H_2(g) respectively.

The rate is then:

$$r = k_3\theta_H\theta_A = K_1\sqrt{K_2}\,k_3P_{H_2}P_A\theta_*^2\,, \tag{S5}$$

The overall KIE ($KIE_{overall}$) is the ratio of rates for the reaction involving H and the reaction involving D:

$$KIE_{overall} = \frac{r_H}{r_D} = \frac{K_{1,H}\sqrt{K_{2,H}}k_{3,H}\theta_{*,H}^2}{K_{1,D}\sqrt{K_{2,D}}k_{3,D}\theta_{*,D}^2} \equiv TIE_1TIE_2KIE_3\frac{\theta_{*,H}^2}{\theta_{*,D}^2} = 1 * TIE_2KIE_3\frac{\theta_{*,H}^2}{\theta_{*,D}^2} \tag{S6}$$

where TIE_i and KIE_i denote the TIE and KIE of elementary step Ei, and subscripts H and D mark quantities evaluated when the H and D isotopes are utilized respectively. TIE_1 is equal to one since elementary step E1 does not involve H. The last term in equation S6—the ratio of the vacant site coverages—does not cancel out since the vacant site coverage depends on K_2, which differs depending on whether H or D is used.

From equation S6, we can see that the overall KIE, which will be the KIE that is experimentally observed, is not just the KIE of elementary step 3, but also crucially contains contributions from the TIEs of elementary steps 1 and 2, as well as contributions from the changes in the amount of vacant sites. The overall experimentally observed KIE is thus a convolution of TIEs and KIEs of the individual elementary steps of the reaction.

S2. Calculation of Thermodynamic Quantities

We calculate the zero-point energy (ZPE) for a system as:

$$ZPE = \frac{hc}{2}\sum_{i}^{m}\frac{1}{\lambda_i}, \tag{S7}$$

where h is the Planck constant, c is the speed of light, m is the number of vibrational modes, and λ_i is the wavelength corresponding to the i-th vibrational mode.

We calculate the vibrational entropy S_{vib} from the harmonic oscillator approximation as:

$$S_{vib} = R\sum_{i}^{m}\left[\frac{x_i}{e^{x_i}-1} - \ln(1-e^{x_i})\right], \tag{S8}$$

where $x_i = \frac{hc}{k_B T}\frac{1}{\lambda_i}$, R is the ideal gas constant, k_B is the Boltzmann constant, T is the reaction temperature, and m is the number of considered vibrational modes.

For adsorption minima, m is equal to $3n$, where n is the number of atoms in the system. For gas-phase species, m is equal to 1. For transition states, m is equal to $3n - 1$, as the mode with the imaginary frequency is not considered.

The entropy of gas-phase species additionally includes: three-dimensional (3D) translational contributions, S_{trans}^{3D}:

$$S_{trans}^{3D} = R\left\{ln\left[\left(\frac{2\pi m k_B T}{h^2}\right)^{\frac{3}{2}}\frac{k_B T}{P}\right] + 2.5\right\}, \tag{S9}$$

where m is the molecular mass, P is the pressure; and rotations, S_{rot}^{linear}:

$$S_{rot}^{linear} = R\left[\ln\left(\frac{8\pi^2 I k_B T}{\sigma h^2}\right) + 1.5\right], \tag{S10}$$

where we have used the formula for linear molecules. I is the principal moment of inertia, and σ is the symmetry number of the molecule (2 for H_2 and D_2).

S3. Thermodynamic and Kinetic Isotope Effects at the Limit of High Temperatures

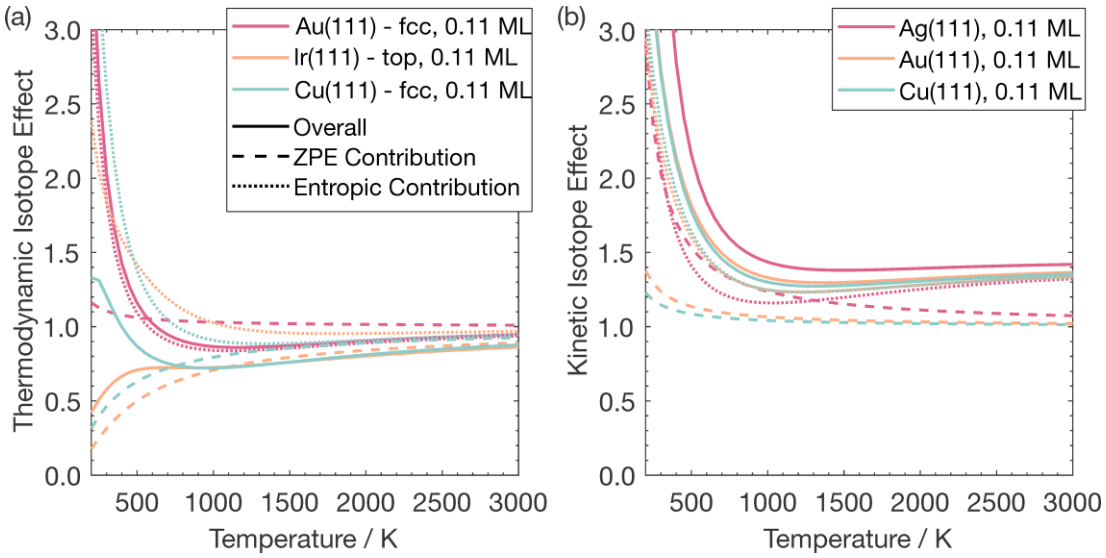

Figure S1 Temperature dependence of the entropic and zero-point energy (ZPE) contributions to the isotope effects of H_2/D_2 dissociative adsorption. (a) Temperature dependence of thermodynamic isotope effects calculated using the most stable low coverage (1/9 ML) H overlayers on Au(111), Ir(111), and Cu(111). (b) Temperature dependence of kinetic isotope effects calculated using the most stable low coverage (2/9 ML) of H_2/D_2 dissociative adsorption transition states on Ag(111), Au(111), and Cu(111).

At the limit of high temperatures, the thermodynamic and kinetic isotope effects (TIEs and KIEs) for H_2/D_2 dissociative adsorption tend to ~1 and ~1.5 respectively (Figure 9 in main text). To understand why, we refer to the expressions for the TIE and KIE as derived in Section 2.3 of the main text, reproduced here for convenience:

$$TIE = \exp\left(-\frac{\Delta ZPE_H - \Delta ZPE_D}{RT}\right)\exp\left(\frac{\Delta S_H - \Delta S_D}{R}\right) \equiv TIE_{ZPE}TIE_{Entropy},$$

$$KIE = \exp\left(-\frac{\Delta ZPE_H^{\ddagger} - \Delta ZPE_D^{\ddagger}}{RT}\right)\exp\left(\frac{\Delta S_H^{\ddagger} - \Delta S_D^{\ddagger}}{R}\right) \equiv KIE_{ZPE}KIE_{Entropy},$$

where ΔZPE is the Zero Point Energy (ZPE) change of reaction, TIE_{ZPE} and $TIE_{Entropy}$ are the ZPE and entropic contributions to the TIE respectively, $\Delta ZPE^{\ddagger}$ is the activation ZPE, and KIE_{ZPE} and $KIE_{Entropy}$ are the ZPE and entropic contributions to the KIE respectively.

Both TIEs and KIEs have two components, namely ZPE and entropic contributions. Figure S1a shows the temperature dependence of the two contributions to the TIE for three example systems where the overall TIE decreases — Au(111), increases — Ir(111), or stays near unity — Cu(111), as the temperature increases; Figure S1b shows the temperature dependence of the two contributions to the KIEs for three close-packed metal surfaces as well — Au(111), Ag(111), and Cu(111).

At the limit of infinite temperature, the ZPE terms of the TIEs and KIEs of all systems tend to unity. This is because as they are proportional to $\exp\left(-\frac{1}{T}\right)$, and the ZPE does not vary with T.

The entropy terms of the TIEs and KIEs decrease with increasing temperature. For the TIEs, the entropy terms tend towards unity at infinite temperature, whereas for the KIEs, the entropy terms tend towards ~1.5. We discuss below the reasons for these trends.

Temperature Dependence of Entropic Contribution to Thermodynamic Isotope Effect

Consider the $\Delta S_H - \Delta S_D$ term in entropic contribution of the TIE, which for a simple H_2 dissociative adsorption reaction on a clean surface can be represented as:

$$\Delta S_H - \Delta S_D = \left(2S_H - S_{H_2}\right) - \left(2S_D - S_{D_2}\right) = 2(S_H - S_D) - (S_{H_2} - S_{D_2}),$$

where S_{H_2}, S_{D_2}, S_H, and S_D are the entropies of gas-phase H_2, gas-phase D_2, adsorbed H and absorbed D respectively.

Whereas the translational and rotational modes of H_2 and D_2 behave classically at very low temperatures, the vibrational modes of all species only begin to behave classically at high temperatures greater than the vibrational temperature (e.g. with a vibrational frequency of 1000cm^{-1}, the vibrational temperature is 1438 K). When the temperature is high enough such that the translation, rotational, and vibration modes all behave classically, both $S_{H_2} - S_{D_2}$ and $S_H - S_D$ tend to a constant, attributable to their different masses. In fact, $S_{H_2} - S_{D_2}$ tends to $2 \times (S_H - S_D)$ as H_2 and 2 H adsorbates both have 6 degrees of freedom. Therefore, $\Delta S_H - \Delta S_D$ tends to zero and the TIE tends to 1: that is, there is no isotope effect as the differences in entropies cancel out.

Temperature Dependence of Entropic Contribution to Kinetic Isotope Effect

We can expand the $\Delta S_H^{\ddagger} - \Delta S_D^{\ddagger}$ term in the entropic contribution of the KIE in a similar way:

$$\Delta S_H^{\ddagger} - \Delta S_D^{\ddagger} = \left(S_H^{\ddagger} - S_{H_2}\right) - \left(S_D^{\ddagger} - S_{D_2}\right) = \left(S_H^{\ddagger} - S_D^{\ddagger}\right) - (S_{H_2} - S_{D_2}),$$

where $S_H^{\ddagger}$ and $S_D^{\ddagger}$ are the entropies of the H- and D-substituted transition states respectively.

In a transition state, however, one vibrational mode is imaginary, so there are only 5 degrees of freedom in the transition state compared with 6 in gas-phase H_2/D_2. The effect of substitution on the entropy of the transition state is thus smaller than that on the gas-phase reactants. $S_H^{\ddagger} - S_D^{\ddagger}$ and $S_{H_2} - S_{D_2}$ are negative quantities, reflecting the higher entropy of the D-substituted reactants, but due to the above effect, $S_H^{\ddagger} - S_D^{\ddagger}$ is more positive than $S_{H_2} - S_{D_2}$. Their difference, $\Delta S_H^{\ddagger} - \Delta S_D^{\ddagger}$, is thus greater than 0 at high temperatures, so the KIEs tend to a value larger than 1, in this case, 1.5.

S4. Supplementary Figures

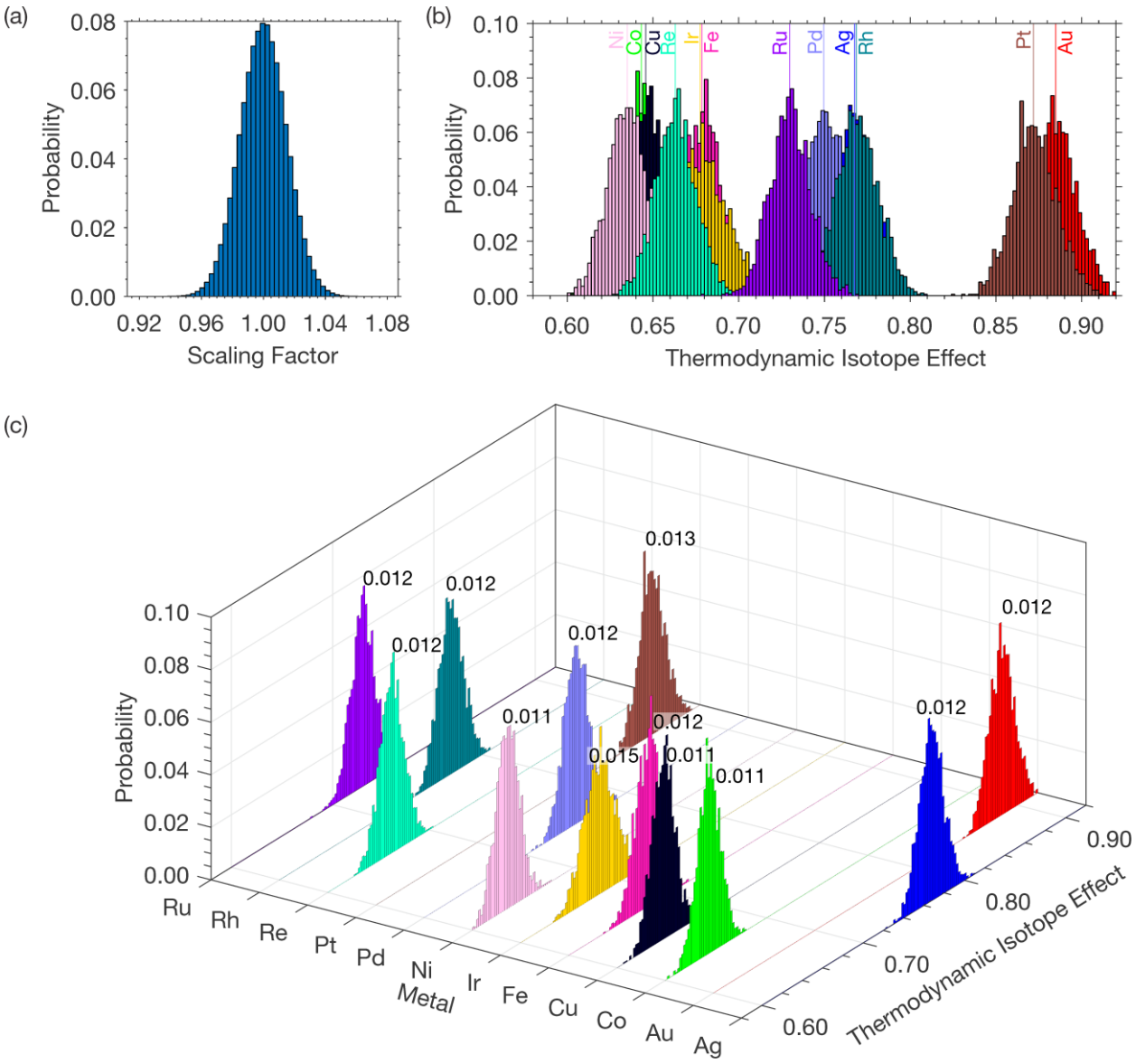

Figure S2 Analysis of effects of errors in vibrational frequencies on calculated thermodynamic isotope effects (TIEs) at 623 K. (a) Frequency scaling factors for simulating errors. (b) Simulated distribution of TIEs of the most stable low coverage (1/9 ML H) structures for each metal. The vibrational frequencies for each structure were scaled using scaling factors randomly drawn from (a) and then used to calculate the TIE. This was repeated 2000 times. Vertical lines mark the TIE calculated without any scaling. (c) The same TIE distribution as in (b) in a waterfall plot to aid in visualization of the different peaks. Numbers near the peaks mark the standard deviation of the normal distribution fitted to each peak.

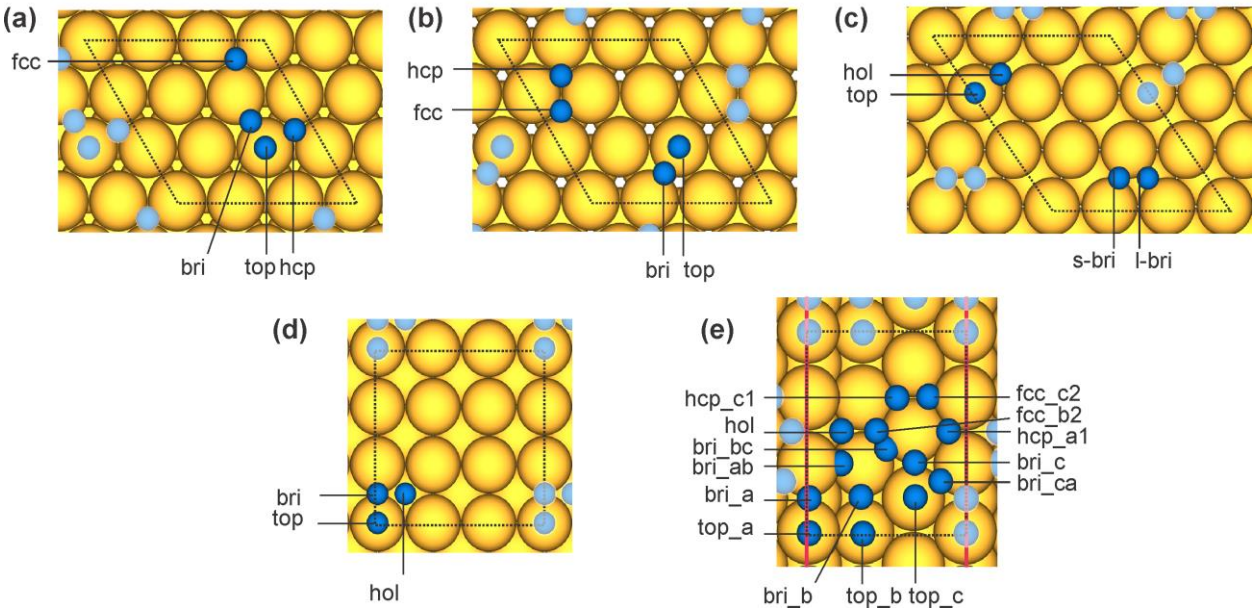

Figure S3 Top view of high-symmetry sites for adsorption of atomic H on (a) fcc (111) surfaces, (b) hcp (0001) surfaces, (c) bcc (110) surfaces, (d) fcc (100) surfaces, and (e) fcc (211) surfaces, where red lines mark the step edges. "hol" and "bri" are abbreviations for "hollow" and "bridge" respectively. Dashed lines mark the unit cell. Color code: yellow – metal, blue – H in unit cell, light blue – H out of unit cell.

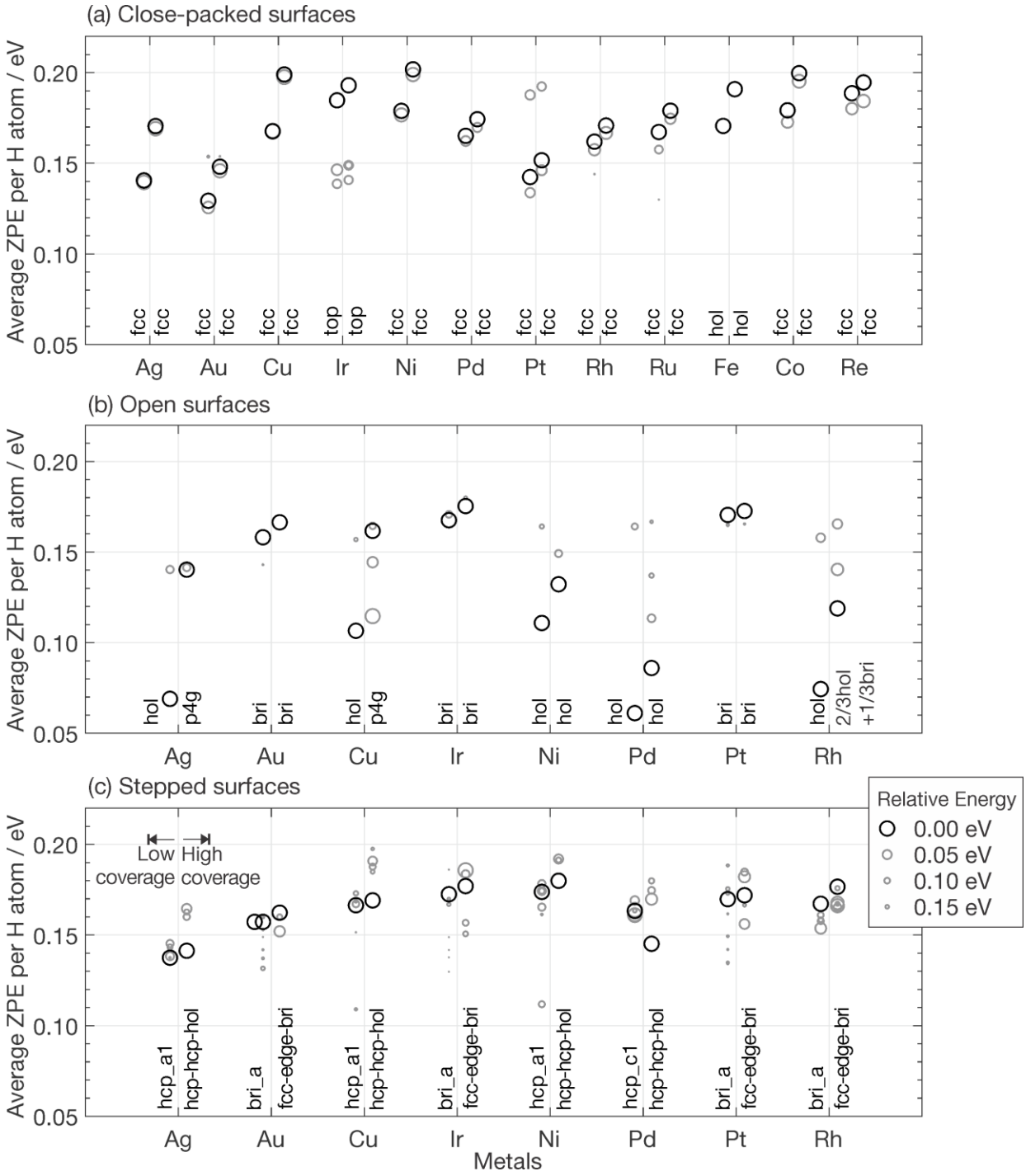

Figure S4 Calculated average zero-point energies (ZPEs) per H atom for H adsorption on (a) close-packed, (b) open, and (c) stepped surfaces Circles mark the TIE for each calculated structure in Tables 1–3 of the main text for the close-packed, open, and stepped surfaces respectively. For each metal, the left-most data points correspond to the low coverage (1/9 ML) ZPEs; the right-most data points correspond to the high coverage (1 ML) ZPEs. Larger circles reflect more stable structures; the circles sizes are based on a Boltzmann distribution at 623 K. The most stable structures for each surface and coverage are highlighted in black and are labelled by their names at the bottom *x*-axis.

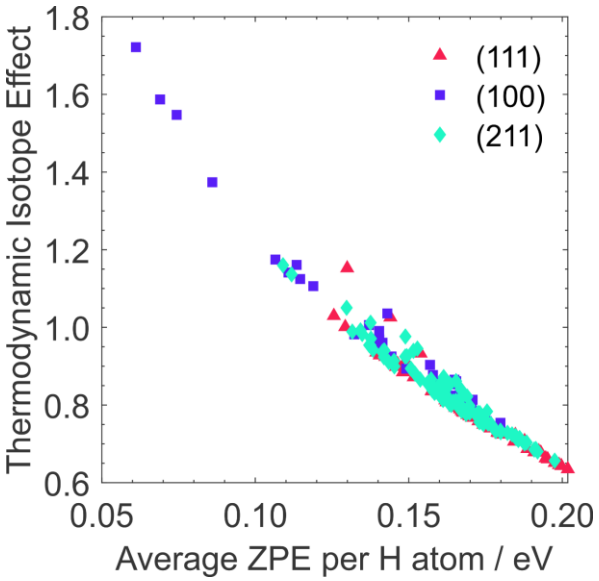

Figure S5 Calculated average zero-point energies (ZPEs) per H atom versus calculated thermodynamic isotope effects (TIEs) for all structures listed in Tables 1–3 of the main text. The TIE's are evaluated at 623 K and 0.1 atm H_2/D_2 pressure.

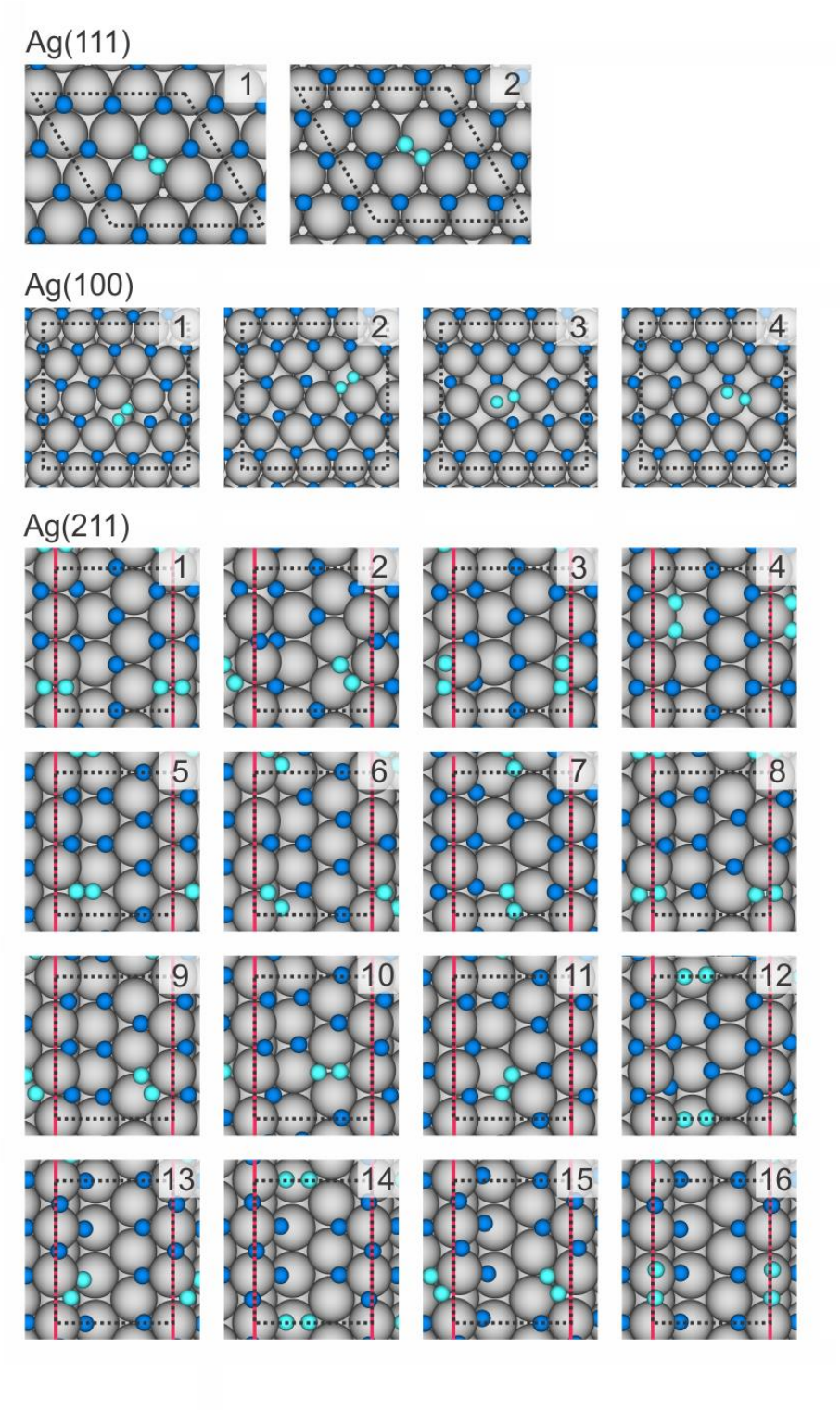

Figure S6 Top views of all identified high-coverage transition state structures for H_2/D_2 dissociative adsorption (initial state 7/9 ML; final state 1 ML) on the (111), (100), and (211) surfaces of Ag. Structures are labelled by their entry numbers in Table S4. Red lines mark the step edges. The unit cell is marked by dashed lines. Color code: grey – Ag, blue – spectator H, cyan – dissociating H_2 molecule.

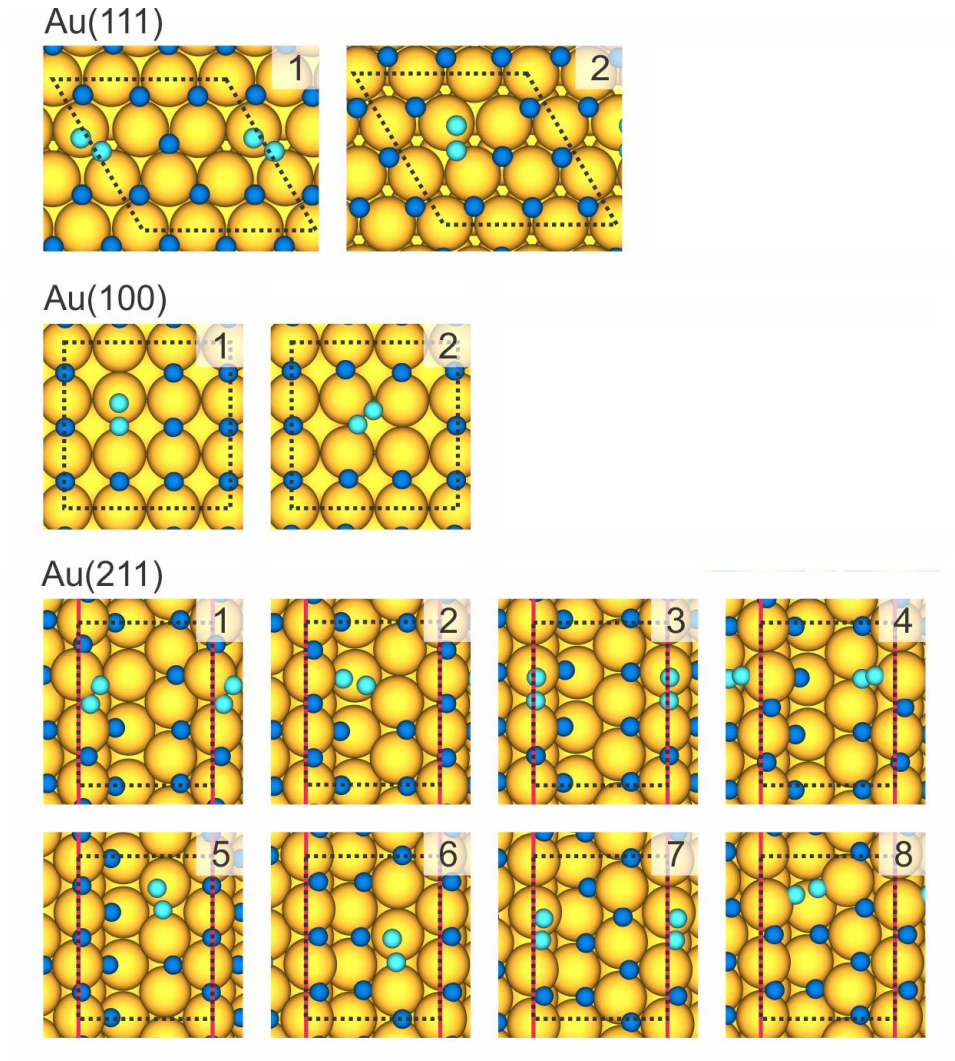

Figure S7 Top views of all identified high-coverage transition state structures for H_2/D_2 dissociative adsorption (initial state 7/9 ML; final state 1 ML) on the (111), (100), and (211) surfaces of Au. Structures are labelled by their entry numbers in Table S4. Red lines mark the step edges. The unit cell is marked by dashed lines. Color code: yellow – Au, blue – spectator H, cyan – dissociating H_2 molecule.

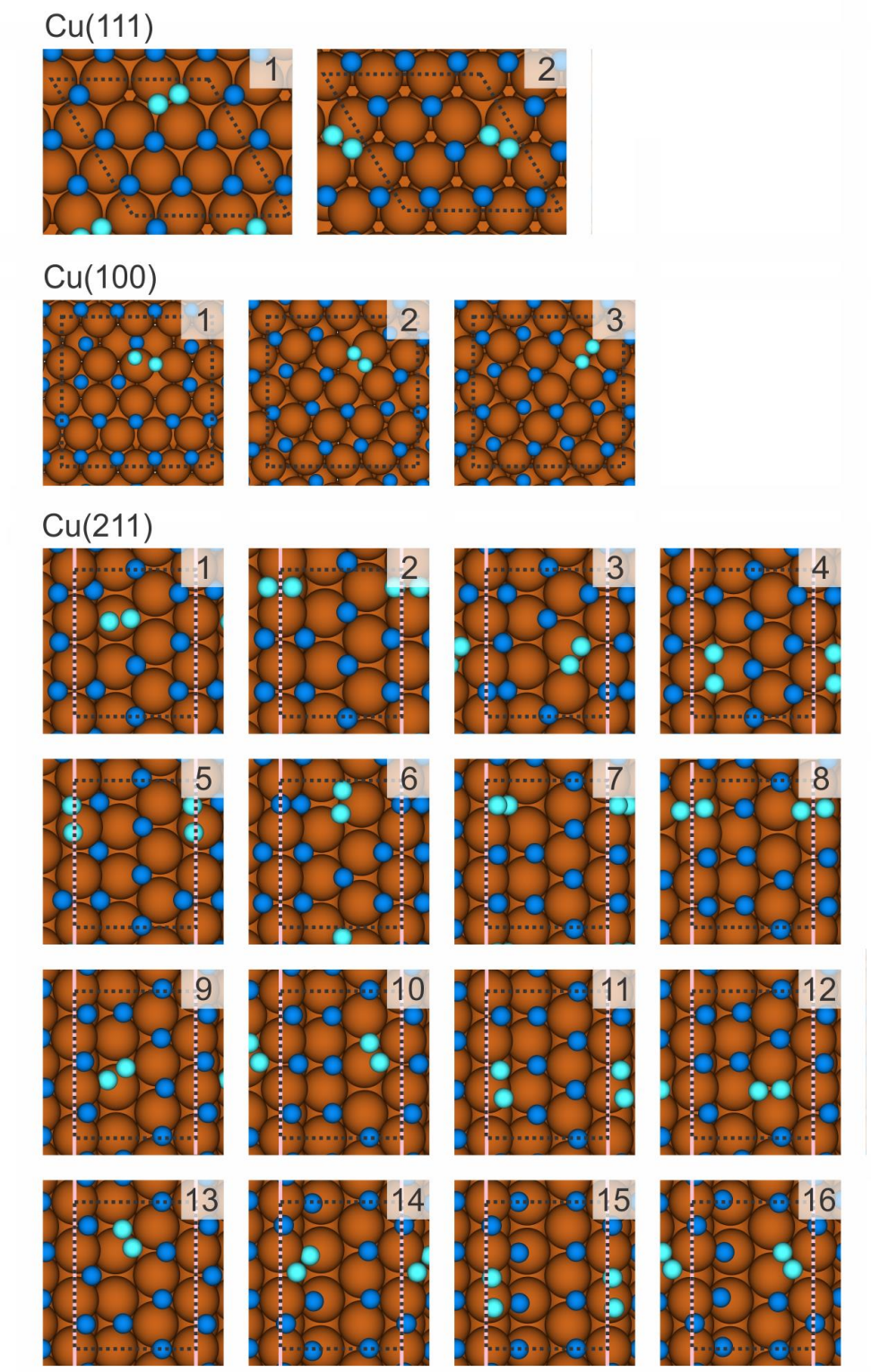

Figure S8 Top views of all identified high-coverage transition state structures for H_2/D_2 dissociative adsorption (initial state 7/9 ML; final state 1 ML) on the (111), (100), and (211) surfaces of Cu. Structures are labelled by their entry numbers in Table S4. Pink lines mark the step edges. The unit cell is marked by dashed lines. Color code: brown – Cu, blue – spectator H, cyan – dissociating H_2 molecule.

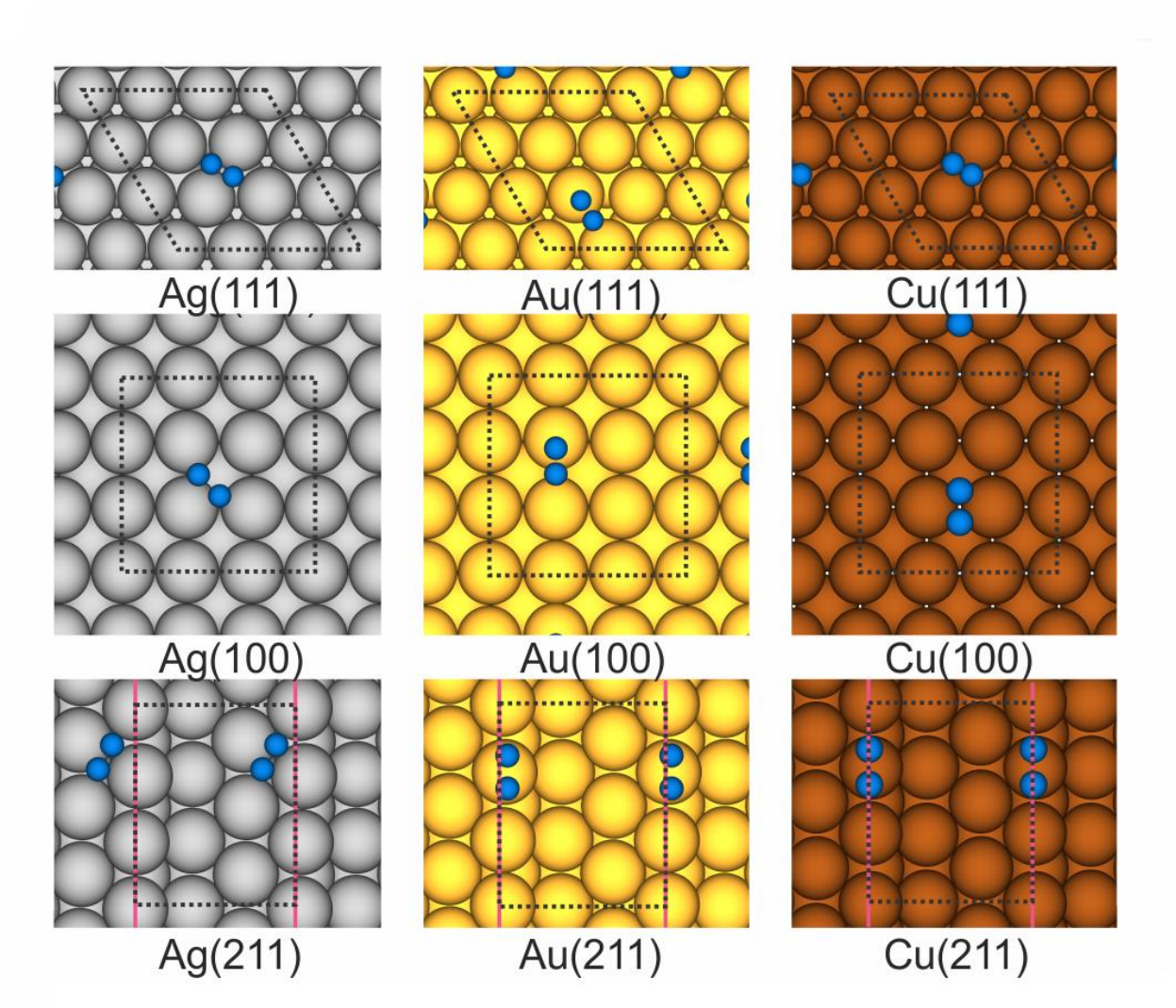

Figure S9 Top views of low-coverage transition state structures for H_2/D_2 dissociative adsorption (initial state 0 ML; final state 2/9 ML) on the (111), (100), and (211) surfaces of Ag, Au, and Cu. Pink lines mark the step edges. The unit cell is marked by dashed lines. Color code: grey – Ag, yellow – Au, brown – Cu, blue – H.

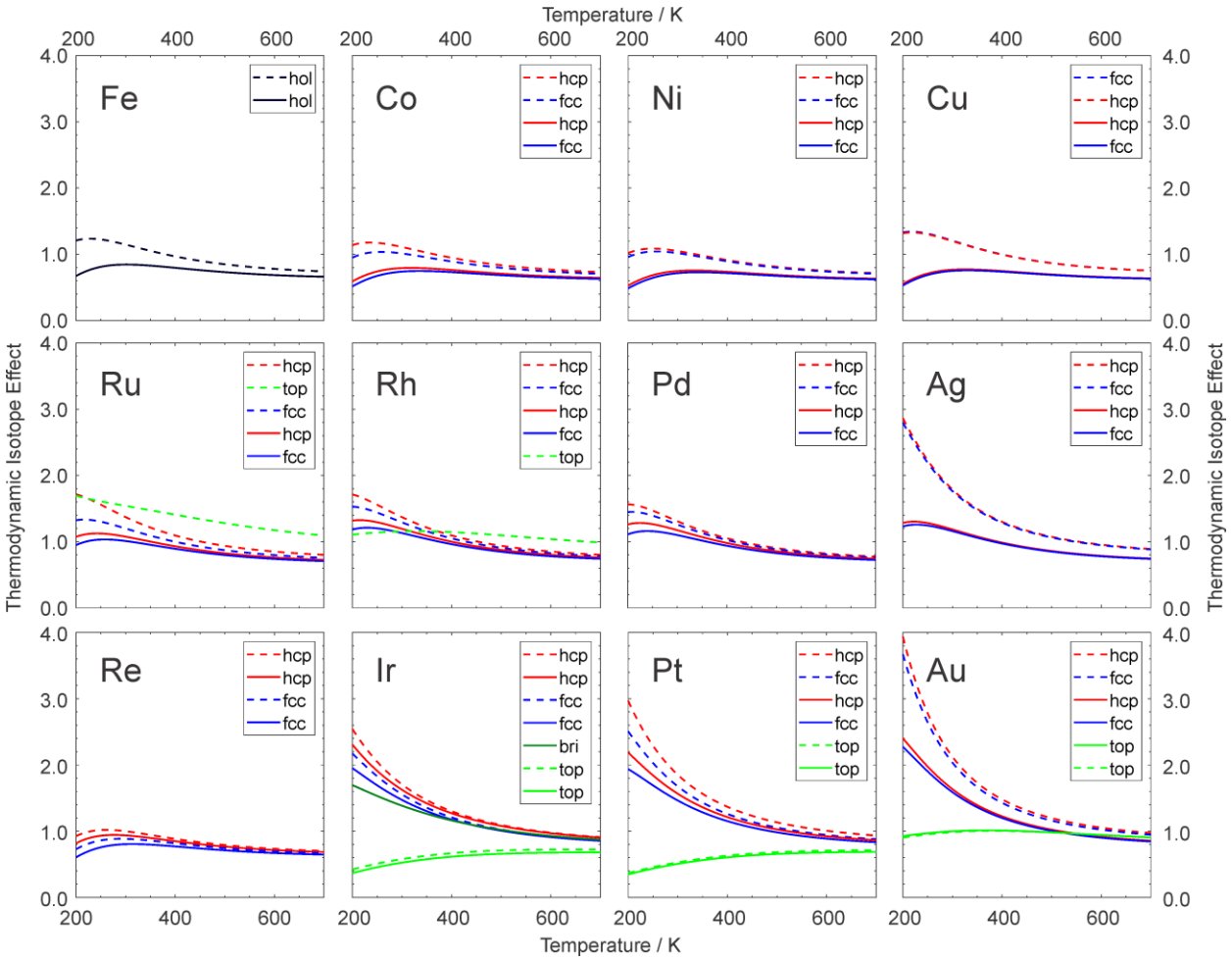

Figure S10 Temperature dependence of thermodynamic isotope effects on close-packed surfaces. Plots are arranged in periodic table order, except for Re. Dashed lines denote low coverage structures whereas full lines denote high coverage structures; these structures are illustrated in Figure S3 and Figure 1 in the main text respectively.

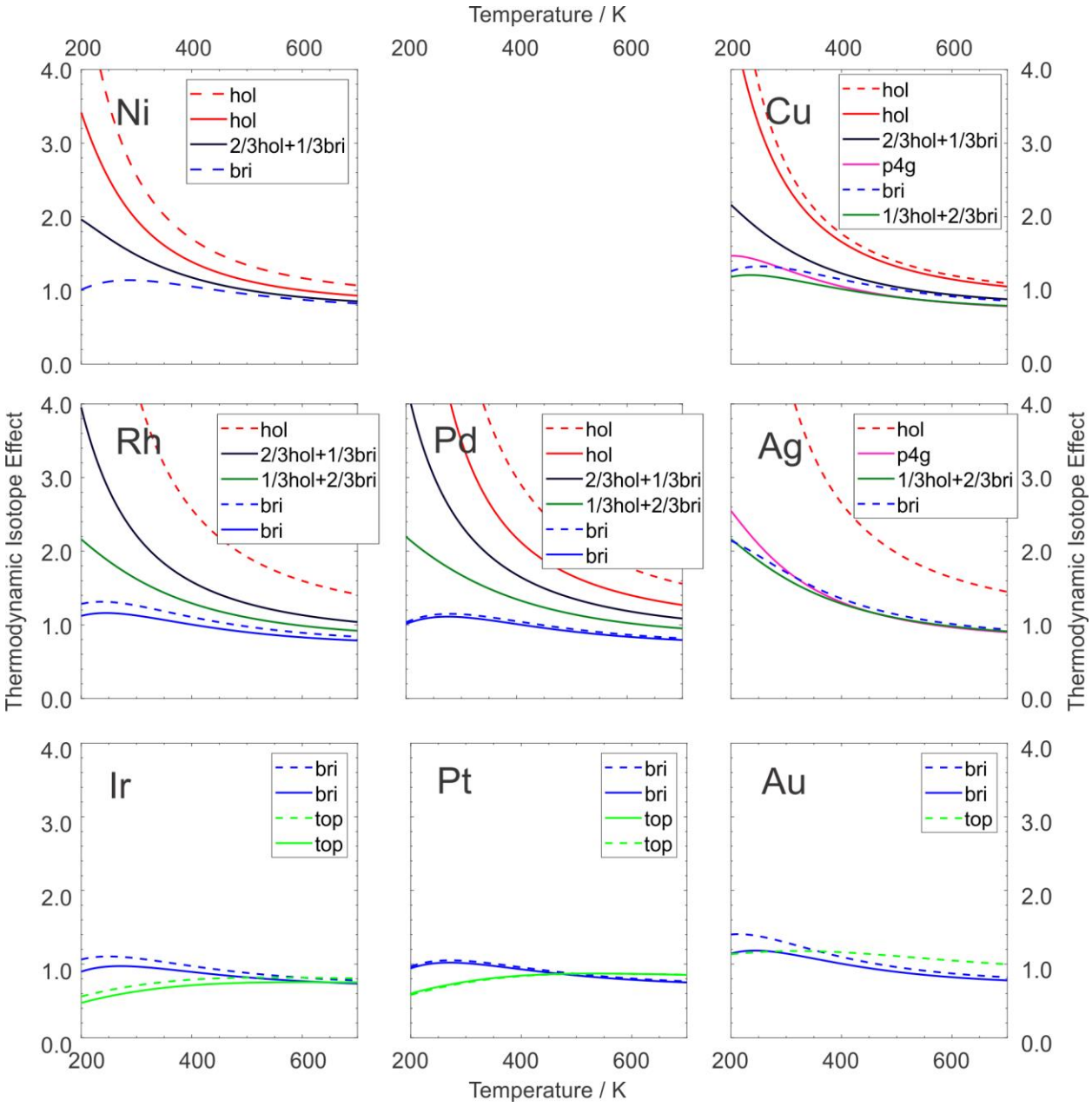

Figure S11 Temperature dependence of thermodynamic isotope effects on open surfaces. Plots are arranged in periodic table order, except for Ni. Dashed lines denote low coverage structures whereas full lines denote high coverage structures; these structures are illustrated in Figure S3 and Figure 3 in the main text respectively.

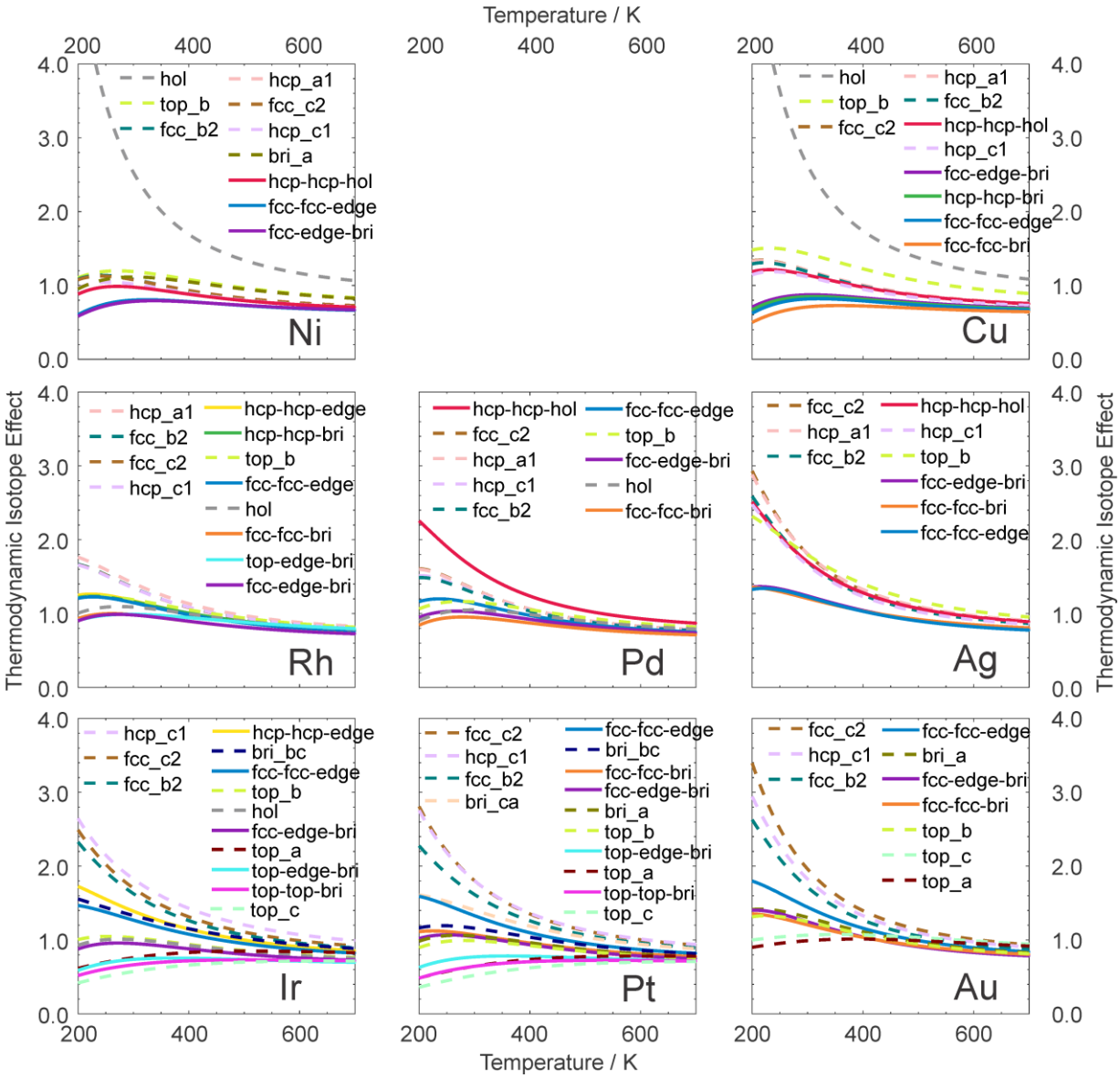

Figure S12 Temperature dependence of thermodynamic isotope effects on stepped surfaces. Dashed lines denote low coverage structures whereas full lines denote high coverage structures; these structures are illustrated in Figure S3 and Figure 5 in the main text respectively.

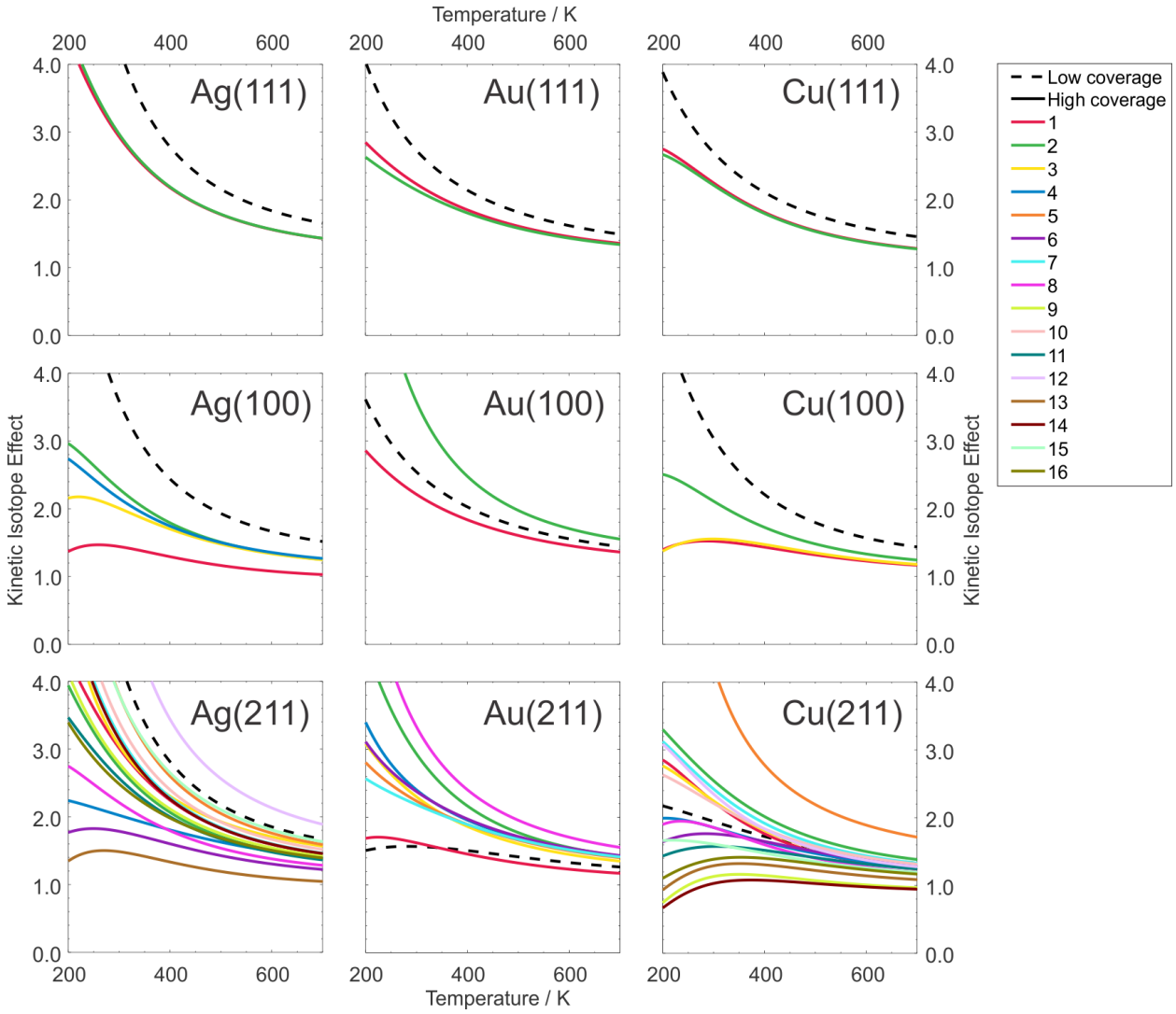

Figure S13 Temperature dependence of kinetic isotope effects on close-packed, open, and stepped surfaces of Ag, Au, and Cu. Dashed lines denote low coverage structures whereas full lines denote high coverage structures. Structures are labelled by their entry numbers in Table S4; and are illustrated in Figure S6-8 for the high-coverage structures, and Figure S9 for the low-coverage structures.

S5. Supplementary Tables

Table S1 Calculated vibrational frequencies (ν, cm^{-1}) for H adsorption on close-packed surfaces. Frequencies for D adsorption can be obtained by dividing those for H by √2.

Surface	Coverage / ML	Structure	ν / cm^{-1}
Ag(111)	0.11	fcc	718, 721, 828
	0.11	hcp	699, 705, 845
	1.00	fcc	800, 800, 810, 810, 810, 810, 811, 811, 869, 886, 889, 919, 919, 921, 921, 921, 922, 975, 975, 1017, 1017, 1017, 1017, 1019, 1020, 1037, 1037
	1.00	hcp	799, 800, 808, 808, 809, 809, 809, 810, 867, 875, 881, 906, 907, 909, 910, 912, 913, 965, 967, 1002, 1004, 1006, 1008, 1008, 1009, 1025, 1025
Au(111)	0.11	fcc	644, 648, 794
	0.11	hcp	593, 596, 837
	0.11	top	244, 247, 1988
	1.00	fcc	632, 644, 678, 678, 681, 682, 689, 690, 802, 805, 807, 807, 814, 815, 816, 816, 820, 821, 873, 873, 885, 885, 885, 886, 888, 888, 943
	1.00	hcp	613, 620, 655, 657, 660, 661, 662, 664, 784, 785, 787, 788, 789, 790, 792, 793, 795, 796, 881, 882, 894, 895, 895, 895, 896, 897, 952
	1.00	top	159, 161, 163, 164, 166, 168, 204, 205, 310, 310, 321, 322, 325, 327, 327, 328, 328, 330, 1948, 1949, 1968, 1969, 1970, 1970, 1970, 1971, 2003
Co(0001)	0.11	fcc	882, 883, 1126
	0.11	hcp	831, 833, 1122
	1.00	fcc	895, 896, 1013, 1014, 1014, 1014, 1015, 1015, 1028, 1029, 1029, 1030, 1030, 1031, 1058, 1058, 1124, 1124, 1156, 1157, 1177, 1178, 1178, 1178, 1179, 1180, 1195
	1.00	hcp	860, 861, 978, 979, 980, 981, 981, 981, 996, 997, 997, 998, 999, 999, 1017, 1018, 1095, 1096, 1151, 1152, 1172, 1173, 1173, 1174, 1174, 1175, 1190
Cu(111)	0.11	fcc	827, 831, 1046
	0.11	hcp	824, 830, 1055
	1.00	fcc	1012, 1012, 1014, 1014, 1022, 1024, 1024, 1024, 1025, 1025, 1026, 1026, 1026, 1027, 1028, 1029, 1077, 1088, 1089, 1149, 1150, 1151, 1151, 1152, 1153, 1186, 1187
	1.00	hcp	1000, 1000, 1011, 1012, 1013, 1013, 1014, 1014, 1015, 1016, 1025, 1026, 1027, 1027, 1027, 1028, 1076, 1079, 1080, 1138, 1138, 1139, 1140, 1140, 1141, 1171, 1172
Fe(110)	0.11	hol	760, 906, 1086
	1.00	hol	856, 856, 902, 902, 902, 902, 915, 915, 942, 995, 995, 996, 996, 996, 997, 1008, 1008, 1019, 1158, 1158, 1182, 1182, 1183, 1183, 1184, 1185, 1194
Ir(111)	0.11	top	402, 405, 2173
	0.11	fcc	615, 619, 1128

	0.11	hcp	547, 552, 1138
	1.00	top	400, 401, 428, 429, 430, 430, 431, 431, 500, 501, 514, 514, 528, 529, 530, 530, 530, 531, 2155, 2156, 2158, 2158, 2158, 2160, 2161, 2162, 2167
	1.00	fcc	545, 546, 554, 559, 581, 581, 583, 583, 586, 586, 605, 605, 608, 609, 609, 609, 697, 697, 1194, 1194, 1208, 1208, 1208, 1209, 1209, 1209, 1233
	1.00	hcp	460, 485, 487, 489, 500, 503, 506, 509, 526, 528, 535, 539, 553, 554, 556, 559, 628, 629, 1195, 1195, 1209, 1210, 1210, 1210, 1211, 1212, 1242
	1.00	bri	179, 359, 361, 362, 362, 522, 523, 532, 533, 580, 582, 584, 584, 585, 586, 619, 661, 662, 1363, 1363, 1369, 1369, 1369, 1369, 1412, 1412, 1424
Ni(111)	0.11	fcc	879, 882, 1125
	0.11	hcp	857, 862, 1131
	1.00	fcc	1001, 1002, 1009, 1009, 1010, 1010, 1011, 1014, 1035, 1036, 1071, 1071, 1071, 1072, 1074, 1074, 1113, 1114, 1144, 1144, 1170, 1170, 1170, 1171, 1172, 1172, 1189
	1.00	hcp	917, 980, 981, 985, 986, 987, 988, 989, 1001, 1004, 1039, 1056, 1057, 1057, 1058, 1059, 1090, 1095, 1141, 1141, 1167, 1167, 1168, 1168, 1169, 1169, 1269
Pd(111)	0.11	fcc	853, 863, 948
	0.11	hcp	828, 837, 953
	1.00	fcc	849, 849, 850, 850, 851, 851, 878, 879, 887, 888, 927, 928, 940, 940, 941, 942, 942, 942, 992, 993, 1023, 1023, 1024, 1024, 1024, 1025, 1046
	1.00	hcp	810, 811, 812, 813, 815, 816, 837, 841, 864, 864, 890, 890, 911, 913, 915, 916, 917, 919, 981, 981, 1013, 1014, 1014, 1014, 1015, 1015, 1047
Pt(111)	0.11	fcc	632, 639, 1026
	0.11	hcp	551, 552, 1055
	0.11	top	381, 385, 2262
	1.00	fcc	608, 608, 610, 611, 612, 613, 625, 628, 688, 689, 700, 702, 715, 716, 717, 719, 720, 721, 1097, 1098, 1113, 1114, 1115, 1115, 1115, 1115, 1132
	1.00	hcp	551, 553, 554, 556, 556, 557, 565, 565, 654, 655, 656, 657, 684, 685, 687, 687, 688, 689, 1097, 1097, 1115, 1115, 1115, 1116, 1116, 1116, 1141
	1.00	top	381, 382, 400, 401, 402, 403, 404, 405, 461, 462, 464, 465, 466, 466, 467, 468, 469, 469, 2227, 2228, 2230, 2231, 2232, 2232, 2233, 2234, 2242
Re(0001)	0.11	fcc	972, 976, 1095
	0.11	hcp	885, 895, 1126
	1.00	fcc	951, 951, 987, 987, 987, 988, 988, 988, 1011, 1011, 1011, 1011, 1011, 1012, 1016, 1017, 1040, 1041, 1120, 1120, 1140, 1140, 1140, 1140, 1140, 1140, 1167
	1.00	hcp	853, 854, 893, 894, 896, 897, 904, 905, 917, 919, 920, 928, 928, 929, 930, 932, 946, 948, 1130, 1130, 1154, 1155, 1155, 1155, 1155, 1155, 1176
Rh(111)	0.11	fcc	760, 764, 1088
	0.11	hcp	727, 730, 1083
	0.11	top	159, 163, 2001

	1.00	fcc	738, 739, 782, 784, 784, 785, 785, 785, 809, 811, 811, 812, 812, 812, 813, 813, 855, 855, 1142, 1143, 1159, 1159, 1159, 1159, 1160, 1177
	1.00	hcp	716, 716, 748, 748, 750, 751, 755, 755, 770, 777, 780, 781, 784, 785, 787, 787, 817, 817, 1138, 1138, 1155, 1155, 1155, 1156, 1156, 1156, 1176
Ru(0001)	0.11	fcc	795, 798, 1105
	0.11	hcp	733, 737, 1072
	0.11	top	105, 124, 1867
	1.00	fcc	776, 777, 856, 857, 858, 858, 859, 860, 876, 879, 881, 883, 883, 884, 884, 885, 930, 930, 1139, 1139, 1154, 1154, 1154, 1154, 1154, 1155, 1171
	1.00	hcp	738, 739, 825, 826, 826, 828, 829, 833, 834, 835, 843, 844, 848, 848, 851, 852, 903, 903, 1136, 1136, 1149, 1149, 1149, 1149, 1150, 1150, 1170

Table S2 Calculated vibrational frequencies (ν, cm^{-1}) for H adsorption on open surfaces. Frequencies for D adsorption can be obtained by dividing those for H by √2.

Surface	Coverage / ML	Structure	ν / cm^{-1}
Ag(100)	0.11	hol	251, 322, 540
	0.11	bri	163, 1013, 1088
	1.00	p4g	217, 232, 237, 247, 284, 355, 359, 391, 633, 651, 687, 696, 697, 700, 703, 707, 716, 722, 724, 726, 746, 765, 778, 792, 819, 850, 855, 861, 862, 869, 875, 878, 895, 902, 906, 914, 918, 925, 932, 940, 984, 996, 1014, 1032, 1041, 1045, 1055, 1075
	1.00	1/3hol+2/3bri	127, 171, 342, 345, 404, 412, 418, 420, 440, 443, 590, 629, 634, 760, 762, 997, 998, 1015, 1016, 1017, 1048, 1222, 1223, 1266, 1267, 1273, 1297
Au(100)	0.11	bri	355, 1059, 1137
	0.11	top	140, 167, 2000
	1.00	bri	320, 321, 327, 474, 475, 475, 476, 477, 477, 1017, 1018, 1085, 1123, 1123, 1124, 1124, 1127, 1128, 1152, 1152, 1152, 1153, 1163, 1163, 1173, 1173, 1188
Cu(100)	0.11	hol	526, 538, 655
	0.11	bri	139, 1173, 1219
	1.00	p4g	447, 449, 457, 458, 459, 463, 469, 490, 741, 765, 767, 769, 772, 802, 804, 835, 837, 859, 861, 876, 883, 884, 884, 930, 949, 960, 962, 964, 967, 969, 971, 986, 991, 1006, 1011, 1012, 1014, 1016, 1037, 1054, 1074, 1091, 1103, 1106, 1121, 1122, 1138, 1145
	1.00	hol	349, 349, 351, 352, 407, 410, 413, 419, 457, 459, 530, 531, 534, 537, 637, 808, 808, 810, 811, 829, 831, 833, 834, 834, 836, 838, 839
	1.00	2/3hol+1/3bri	318, 416, 419, 476, 477, 509, 533, 548, 574, 593, 596, 622, 625, 625, 836, 851, 852, 892, 893, 897, 898, 1184, 1184, 1219, 1288, 1290, 1348
	1.00	1/3hol+2/3bri	75, 178, 453, 455, 533, 542, 547, 560, 564, 639, 758, 786, 787, 921, 924, 1187, 1188, 1213, 1214, 1217, 1235, 1288, 1289, 1320, 1321, 1341, 1343
Ir(100)	0.11	bri	418, 903, 1382
	0.11	top	295, 312, 2148
	1.00	bri	477, 501, 503, 548, 548, 549, 549, 550, 552, 864, 864, 866, 867, 867, 870, 904, 906, 907, 1406, 1407, 1407, 1407, 1411, 1412, 1438, 1438, 1444
	1.00	top	263, 264, 265, 267, 268, 270, 425, 427, 428, 429, 430, 430, 431, 432, 435, 436, 438, 438, 2146, 2147, 2148, 2148, 2148, 2149, 2149, 2150, 2152
Ni(100)	0.11	hol	524, 536, 728
	0.11	bri	163, 1163, 1321
	1.00	hol	594, 595, 596, 596, 635, 636, 637, 637, 684, 685, 693, 695, 696, 697, 698, 772, 774, 775, 775, 786, 786, 787, 788, 793, 794, 796, 797
	1.00	2/3hol+1/3bri	176, 483, 504, 593, 598, 622, 624, 634, 664, 696, 703, 703, 713, 714, 755, 780, 784, 788, 790, 797, 798, 1242, 1249, 1277, 1315, 1318, 1336

Pd(100)	0.11	hol	70, 370, 546
	0.11	bri	202, 1213, 1232
	1.00	hol	355, 359, 363, 367, 370, 376, 440, 441, 447, 448, 452, 454, 458, 459, 460, 464, 465, 467, 501, 506, 509, 513, 513, 572, 573, 576, 579
	1.00	2/3hol+1/3bri	102, 298, 303, 375, 381, 400, 403, 405, 420, 433, 436, 437, 439, 441, 465, 492, 495, 499, 585, 586, 591, 1203, 1203, 1211, 1282, 1285, 1305
	1.00	1/3hol+2/3bri	112, 180, 288, 291, 307, 314, 348, 352, 399, 407, 412, 428, 434, 480, 488, 1171, 1172, 1187, 1195, 1196, 1204, 1216, 1218, 1231, 1281, 1283, 1302
	1.00	bri	146, 218, 222, 321, 322, 328, 330, 332, 334, 1145, 1147, 1149, 1152, 1155, 1159, 1162, 1183, 1191, 1238, 1240, 1242, 1244, 1244, 1245, 1246, 1253, 1255
Pt(100)	0.11	bri	389, 1040, 1321
	0.11	top	203, 212, 2245
	1.00	bri	391, 422, 425, 467, 469, 470, 472, 475, 478, 955, 956, 961, 975, 977, 979, 981, 1004, 1007, 1344, 1345, 1346, 1346, 1349, 1350, 1372, 1373, 1377
	1.00	top	93, 95, 101, 105, 108, 111, 272, 276, 278, 278, 279, 283, 284, 286, 292, 293, 294, 297, 2221, 2221, 2221, 2221, 2222, 2222, 2223, 2223, 2226
Rh(100)	0.11	hol	218, 253, 729
	0.11	bri	245, 1002, 1300
	1.00	2/3hol+1/3bri	285, 357, 376, 378, 395, 398, 410, 418, 421, 422, 452, 456, 458, 462, 465, 669, 670, 691, 692, 697, 722, 1010, 1011, 1021, 1306, 1306, 1313
	1.00	1/3hol+2/3bri	238, 259, 265, 272, 315, 422, 426, 429, 430, 432, 455, 464, 712, 727, 750, 954, 955, 967, 995, 996, 1000, 1306, 1306, 1313, 1330, 1331, 1336
	1.00	bri	264, 321, 323, 431, 432, 433, 434, 435, 436, 926, 927, 928, 928, 937, 939, 988, 991, 992, 1316, 1317, 1317, 1318, 1322, 1323, 1348, 1348, 1353

Table S3 Calculated vibrational frequencies (ν, cm^{-1}) for H adsorption on stepped surfaces. Frequencies for D adsorption can be obtained by dividing those for H by √2.

Surface	Coverage / ML	Structure	ν / cm^{-1}
Ag(211)	0.11	hcp_a1	526, 807, 885
	0.11	fcc_c2	668, 712, 852
	0.11	hcp_c1	727, 782, 835
	0.11	fcc_b2	703, 759, 852
	0.11	top_b	144, 1025, 1050
	1.00	hcp-hcp-hol	372, 379, 380, 475, 533, 534, 591, 644, 645, 657, 698, 698, 778, 778, 799, 883, 898, 898, 909, 934, 961, 963, 1001, 1001, 1012, 1050, 1051
	1.00	fcc-fcc-edge	281, 285, 324, 748, 749, 757, 771, 771, 789, 895, 896, 907, 931, 952, 960, 961, 1005, 1020, 1021, 1035, 1036, 1071, 1071, 1100, 1160, 1195, 1198
	1.00	fcc-fcc-bri	303, 399, 405, 452, 481, 486, 557, 613, 614, 696, 697, 709, 782, 811, 823, 829, 882, 887, 1042, 1043, 1059, 1160, 1162, 1175, 1719, 1722, 1726
	1.00	fcc-edge-bri	362, 364, 391, 397, 507, 510, 784, 786, 798, 891, 900, 903, 926, 970, 972, 990, 994, 1005, 1026, 1026, 1058, 1075, 1135, 1138, 1221, 1227, 1267
Au(211)	0.11	bri_a	329, 1094, 1114
	0.11	fcc_c2	592, 652, 879
	0.11	top_b	345, 1043, 1191
	0.11	hcp_c1	555, 777, 880
	0.11	fcc_b2	639, 715, 935
	0.11	top_a	195, 255, 2015
	0.11	top_c	200, 217, 1985
	1.00	fcc-edge-bri	434, 436, 462, 542, 594, 594, 686, 692, 700, 750, 846, 851, 862, 867, 881, 970, 1024, 1025, 1042, 1094, 1095, 1137, 1139, 1192, 1214, 1217, 1225
	1.00	fcc-fcc-edge	317, 320, 340, 401, 403, 404, 732, 748, 750, 755, 817, 818, 822, 823, 848, 857, 962, 964, 1010, 1014, 1054, 1063, 1148, 1152, 1167, 1169, 1214
	1.00	fcc-fcc-bri	303, 399, 405, 452, 481, 486, 557, 613, 614, 696, 697, 709, 782, 811, 823, 829, 882, 887, 1042, 1043, 1059, 1160, 1162, 1175, 1719, 1722, 1726
Cu(211)	0.11	hcp_a1	669, 920, 1096
	0.11	fcc_c2	797, 814, 1086
	0.11	hcp_c1	840, 898, 1053
	0.11	fcc_b2	790, 896, 1035
	0.11	hol	416, 632, 711
	0.11	top_b	111, 1101, 1232
	1.00	hcp-hcp-hol	464, 473, 530, 623, 643, 648, 701, 813, 824, 828, 854, 858, 970, 971, 988, 1009, 1029, 1061, 1063, 1095, 1119, 1120, 1137, 1138, 1195, 1198, 1206

	1.00	fcc-fcc-edge	412, 417, 430, 937, 940, 962, 997, 998, 1000, 1020, 1031, 1040, 1043, 1070, 1072, 1074, 1116, 1118, 1131, 1140, 1142, 1233, 1235, 1279, 1288, 1292, 1294
	1.00	hcp-hcp-bri	202, 454, 456, 803, 806, 841, 966, 966, 977, 1006, 1035, 1037, 1057, 1058, 1059, 1060, 1101, 1103, 1112, 1115, 1134, 1158, 1181, 1182, 1457, 1458, 1471
	1.00	fcc-edge-bri	363, 428, 430, 466, 582, 584, 950, 952, 960, 1042, 1042, 1048, 1075, 1111, 1112, 1137, 1141, 1141, 1170, 1203, 1206, 1226, 1228, 1246, 1328, 1330, 1352
	1.00	fcc-fcc-bri	378, 565, 566, 852, 869, 871, 877, 879, 891, 922, 960, 960, 1015, 1026, 1028, 1042, 1120, 1121, 1260, 1261, 1263, 1359, 1360, 1397, 1609, 1609, 1621
Ir(211)	0.11	bri_a	432, 973, 1378
	0.11	top_a	257, 312, 2124
	0.11	top_b	466, 842, 1433
	0.11	top_c	403, 443, 2156
	0.11	hcp_c1	299, 495, 1299
	0.11	bri_bc	316, 604, 1481
	0.11	fcc_c2	451, 583, 1187
	0.11	fcc_b2	496, 625, 1166
	1.00	fcc-edge-bri	492, 495, 544, 578, 639, 642, 649, 662, 664, 669, 702, 706, 904, 905, 935, 1032, 1035, 1036, 1207, 1208, 1213, 1402, 1403, 1436, 1512, 1515, 1517
	1.00	top-edge-bri	441, 463, 464, 481, 488, 488, 500, 518, 519, 583, 641, 641, 918, 918, 941, 946, 955, 958, 1404, 1405, 1434, 1460, 1461, 1463, 2155, 2156, 2161
	1.00	top-top-bri	287, 388, 392, 418, 421, 440, 441, 469, 471, 472, 476, 501, 503, 526, 539, 778, 823, 827, 1518, 1524, 1526, 2149, 2150, 2154, 2155, 2156, 2159
	1.00	fcc-fcc-edge	393, 436, 438, 500, 526, 527, 530, 545, 546, 567, 574, 574, 576, 645, 646, 918, 921, 947, 1219, 1220, 1238, 1333, 1334, 1340, 1408, 1411, 1445
	1.00	hcp-hcp-edge	372, 399, 404, 453, 475, 477, 499, 511, 517, 527, 554, 561, 692, 695, 697, 777, 779, 814, 1208, 1213, 1220, 1232, 1233, 1252, 1421, 1422, 1467
Ni(211)	0.11	hcp_a1	719, 926, 1159
	0.11	fcc_c2	819, 831, 1162
	0.11	hcp_c1	858, 859, 1160
	0.11	bri_a	128, 1227, 1313
	0.11	hol	452, 593, 759
	0.11	fcc_b2	802, 888, 1122
	0.11	top_b	176, 1081, 1346
	1.00	hcp-hcp-hol	488, 493, 496, 848, 855, 856, 868, 904, 905, 913, 917, 940, 971, 978, 1006, 1030, 1047, 1072, 1076, 1102, 1104, 1177, 1180, 1197, 1220, 1222, 1259
	1.00	fcc-fcc-edge	419, 443, 446, 936, 940, 941, 996, 997, 999, 1000, 1030, 1031, 1035, 1048, 1050, 1125, 1125, 1138, 1155, 1155, 1171, 1207, 1211, 1271, 1322, 1323, 1357
	1.00	fcc-edge-bri	367, 450, 456, 518, 610, 615, 922, 928, 950, 1046, 1087, 1092, 1144, 1151, 1165, 1166, 1169, 1224, 1228, 1229, 1230, 1316, 1317, 1344, 1348, 1348, 1363
Pd(211)	0.11	hcp_c1	821, 830, 983

	0.11	fcc_b2	781, 874, 988
	0.11	hcp_a1	719, 926, 951
	0.11	fcc_c2	807, 834, 959
	0.11	bri_a	240, 1206, 1281
	0.11	top_b	214, 1168, 1255
	1.00	hcp-hcp-hol	338, 340, 368, 538, 544, 563, 568, 575, 607, 766, 768, 797, 847, 875, 888, 894, 915, 918, 944, 944, 949, 978, 978, 1006, 1041, 1045, 1087
	1.00	fcc-fcc-edge	343, 386, 392, 830, 835, 838, 848, 849, 850, 879, 900, 913, 916, 938, 939, 967, 968, 973, 974, 991, 1001, 1121, 1124, 1157, 1236, 1238, 1248
	1.00	fcc-edge-bri	385, 392, 394, 456, 528, 531, 755, 756, 783, 911, 973, 978, 1008, 1011, 1039, 1102, 1102, 1119, 1173, 1175, 1180, 1224, 1225, 1256, 1296, 1297, 1304
	1.00	fcc-fcc-bri	350, 403, 412, 792, 793, 829, 833, 852, 853, 854, 890, 892, 895, 944, 948, 1066, 1066, 1080, 1105, 1107, 1115, 1173, 1175, 1205, 1492, 1493, 1498
Pt(211)	0.11	bri_a	382, 1048, 1309
	0.11	top_a	294, 331, 2206
	0.11	top_b	409, 1004, 1380
	0.11	top_c	377, 393, 2269
	0.11	fcc_c2	508, 561, 1106
	0.11	bri_ca	245, 802, 1362
	0.11	hcp_c1	432, 596, 1138
	0.11	fcc_b2	458, 656, 1178
	0.11	bri_bc	309, 894, 1406
	1.00	fcc-edge-bri	488, 490, 534, 538, 541, 547, 569, 621, 622, 695, 771, 772, 947, 957, 960, 1111, 1113, 1126, 1127, 1129, 1139, 1326, 1327, 1359, 1380, 1382, 1393
	1.00	top-edge-bri	373, 408, 411, 418, 437, 441, 466, 468, 500, 513, 583, 586, 918, 922, 926, 1109, 1109, 1124, 1314, 1315, 1319, 1333, 1334, 1369, 2248, 2250, 2254
	1.00	fcc-fcc-edge	444, 464, 467, 477, 480, 495, 513, 620, 621, 662, 690, 691, 744, 754, 755, 964, 966, 977, 1107, 1107, 1131, 1159, 1162, 1168, 1334, 1335, 1372
	1.00	top-top-bri	280, 371, 387, 390, 407, 409, 412, 423, 425, 429, 439, 443, 446, 475, 481, 1031, 1031, 1051, 1381, 1381, 1383, 2190, 2192, 2198, 2256, 2257, 2261
	1.00	fcc-fcc-bri	371, 462, 467, 555, 557, 559, 594, 598, 601, 618, 661, 664, 702, 704, 706, 804, 829, 830, 1175, 1176, 1195, 1388, 1390, 1401, 1721, 1724, 1728
Rh(211)	0.11	bri_a	306, 1083, 1309
	0.11	hcp_a1	502, 867, 1111
	0.11	hcp_c1	672, 730, 1142
	0.11	top_b	316, 926, 1356
	0.11	fcc_b2	704, 751, 1098
	0.11	fcc_c2	724, 733, 1099
	1.00	fcc-edge-bri	428, 429, 477, 480, 584, 585, 780, 780, 807, 815, 836, 837, 974, 975, 1032, 1055, 1070, 1071, 1131, 1132, 1140, 1329, 1330, 1356, 1404, 1405, 1408

1.00	hcp-hcp-edge	325, 372, 376, 718, 719, 741, 753, 761, 761, 767, 780, 781, 848, 849, 898, 930, 931, 960, 1107, 1108, 1117, 1156, 1156, 1172, 1332, 1333, 1375
1.00	fcc-fcc-edge	409, 437, 438, 694, 697, 722, 742, 766, 769, 785, 786, 794, 807, 814, 816, 977, 980, 1024, 1141, 1141, 1148, 1148, 1156, 1170, 1320, 1320, 1352
1.00	hcp-hcp-bri	180, 327, 331, 586, 590, 609, 685, 689, 701, 804, 806, 812, 852, 853, 869, 958, 960, 964, 1153, 1155, 1175, 1178, 1178, 1200, 1459, 1464, 1468
1.00	fcc-fcc-bri	422, 485, 486, 700, 731, 734, 739, 741, 762, 787, 789, 806, 819, 824, 824, 898, 902, 903, 1201, 1202, 1224, 1300, 1301, 1309, 1543, 1548, 1549
1.00	top-edge-bri	96, 229, 232, 258, 314, 317, 397, 399, 430, 436, 549, 551, 950, 951, 987, 1026, 1027, 1027, 1326, 1326, 1347, 1361, 1362, 1368, 2005, 2007, 2011

Table S4 Calculated vibrational frequencies (ν, cm^{-1}) for transition states of H_2 dissociative adsorption on close-packed surfaces. Frequencies for D_2 dissociative adsorption can be obtained by dividing those for H_2 by $\sqrt{2}$. Illustrations of the high coverage (1.00 ML) transition states can be found in Figure S6-8 for the Ag, Au, and Cu surfaces respectively, whereas illustrations of the low coverage transition states (0.22 ML) can be found in Figure S9.

Surface	Coverage / ML	Entry No.	ν, cm^{-1}
Ag(111)	0.22	1	354, 556, 724, 822, 847
	1.00	1	345, 523, 724, 751, 776, 790, 797, 803, 814, 828, 847, 859, 873, 886, 901, 916, 943, 946, 972, 986, 1009, 1012, 1037, 1044, 1085, 1167
		2	371, 535, 710, 745, 780, 791, 794, 800, 819, 822, 844, 847, 870, 881, 890, 906, 933, 938, 959, 976, 997, 999, 1024, 1031, 1068, 1146
Au(111)	0.22	1	293, 407, 595, 928, 1789
	1.00	1	301, 411, 503, 580, 596, 618, 660, 676, 719, 735, 756, 777, 787, 804, 815, 816, 840, 855, 904, 934, 939, 948, 978, 1020, 1068, 1768
		2	306, 418, 500, 559, 565, 584, 616, 642, 695, 708, 737, 754, 765, 790, 792, 805, 831, 878, 929, 935, 963, 970, 982, 1008, 1048, 1766
Cu(111)	0.22	1	345, 385, 767, 968, 1655
	1.00	1	490, 648, 818, 891, 913, 922, 972, 975, 992, 1006, 1016, 1029, 1033, 1043, 1052, 1057, 1069, 1080, 1114, 1120, 1143, 1148, 1168, 1186, 1212, 1273
		2	483, 650, 810, 887, 899, 917, 966, 976, 990, 1002, 1013, 1027, 1036, 1044, 1051, 1054, 1062, 1077, 1112, 1113, 1134, 1138, 1159, 1177, 1203, 1270
Ag(100)	0.22	1	616, 626, 716, 792, 974
	1.00	1	351, 382, 403, 451, 491, 509, 518, 552, 572, 585, 597, 611, 627, 628, 639, 659, 662, 694, 711, 725, 776, 787, 811, 841, 848, 871, 879, 882, 890, 900, 903, 911, 927, 935, 945, 967, 981, 986, 999, 1017, 1019, 1026, 1044, 1077, 1080, 1184, 1244
		2	316, 369, 396, 402, 414, 477, 502, 530, 550, 570, 578, 585, 596, 640, 659, 661, 681, 703, 721, 737, 761, 816, 834, 845, 856, 861, 868, 885, 891, 906, 909, 918, 924, 932, 948, 957, 967, 979, 991, 1001, 1007, 1015, 1032, 1042, 1048, 1089, 1172
		3	78, 158, 252, 359, 401, 448, 485, 514, 560, 564, 641, 653, 657, 669, 694, 700, 707, 714, 718, 730, 756, 771, 819, 820, 847, 852, 861, 874, 888, 895, 909, 912, 937, 943, 951, 963, 973, 995, 1000, 1002, 1015, 1029, 1056, 1059, 1067, 1173, 1595
		4	217, 313, 326, 367, 394, 416, 432, 547, 558, 595, 609, 635, 642, 657, 667, 685, 700, 705, 729, 731, 742, 782, 784, 821, 834, 853, 870, 874, 886, 898, 904, 912, 926, 930, 959, 961, 972, 990, 998, 1008, 1013, 1027, 1035, 1072, 1075, 1237, 1565
Au(100)	0.22	1	320, 449, 679, 920, 1808
	1.00	1	267, 319, 359, 395, 439, 467, 470, 476, 546, 620, 1001, 1010, 1046, 1088, 1102, 1105, 1113, 1118, 1143, 1148, 1152, 1158, 1163, 1184, 1187, 1857
		2	330, 363, 376, 430, 455, 461, 471, 490, 508, 577, 978, 1001, 1021, 1033, 1068, 1097, 1105, 1114, 1116, 1117, 1134, 1154, 1165, 1180, 1199, 1218

Cu(100)	0.22	1	440, 630, 874, 990, 1133
	1.00	1	284, 367, 386, 489, 516, 545, 611, 622, 644, 696, 727, 754, 781, 797, 815, 832, 850, 874, 884, 904, 909, 939, 943, 948, 956, 966, 975, 985, 992, 1005, 1018, 1028, 1031, 1035, 1049, 1061, 1070, 1093, 1102, 1104, 1120, 1149, 1156, 1165, 1205, 1427, 1684
		2	388, 405, 459, 480, 548, 560, 564, 584, 595, 699, 718, 724, 779, 789, 805, 819, 836, 849, 860, 872, 884, 896, 915, 922, 926, 930, 938, 942, 944, 954, 976, 979, 997, 1005, 1021, 1024, 1043, 1058, 1061, 1071, 1087, 1102, 1117, 1229, 1264, 1305, 1372
		3	227, 418, 439, 449, 481, 490, 523, 576, 663, 690, 756, 764, 790, 794, 816, 822, 845, 859, 877, 891, 895, 910, 912, 923, 933, 939, 954, 963, 969, 971, 982, 986, 992, 998, 1001, 1026, 1035, 1061, 1072, 1102, 1109, 1136, 1150, 1159, 1294, 1396, 1480
Ag(211)	0.22	1	403, 552, 664, 779, 855
	1.00	1	230, 291, 350, 446, 551, 574, 645, 716, 755, 757, 777, 799, 817, 866, 897, 916, 919, 924, 933, 955, 958, 991, 999, 1032, 1038, 1043
		2	192, 297, 401, 484, 548, 594, 682, 695, 717, 738, 746, 771, 798, 833, 844, 873, 887, 910, 928, 951, 992, 1007, 1063, 1100, 1202, 1305
		3	216, 242, 350, 441, 497, 530, 607, 633, 651, 692, 754, 772, 796, 838, 872, 882, 916, 927, 938, 949, 975, 998, 1026, 1329, 1411, 1690
		4	64, 175, 283, 409, 424, 584, 687, 739, 759, 780, 789, 795, 836, 845, 868, 883, 889, 909, 940, 967, 972, 991, 1176, 1189, 1709, 1764
		5	226, 325, 359, 593, 660, 731, 757, 772, 775, 799, 807, 845, 877, 930, 930, 935, 946, 969, 970, 1014, 1025, 1026, 1091, 1105, 1149, 1186
		6	375, 421, 473, 712, 732, 734, 751, 757, 790, 810, 831, 878, 914, 934, 952, 980, 985, 1004, 1005, 1013, 1039, 1074, 1126, 1176, 1197, 1492
		7	48, 324, 341, 438, 460, 555, 561, 601, 653, 659, 671, 699, 745, 745, 761, 812, 847, 878, 892, 896, 913, 955, 1002, 1016, 1066, 1134
		8	330, 362, 403, 637, 717, 753, 759, 768, 786, 817, 831, 845, 863, 896, 919, 963, 965, 987, 1029, 1034, 1055, 1064, 1129, 1182, 1303, 1356
		9	303, 351, 361, 571, 736, 747, 770, 786, 810, 823, 834, 837, 875, 886, 895, 900, 961, 997, 1027, 1029, 1048, 1057, 1101, 1250, 1268, 1285
		10	296, 321, 345, 400, 549, 609, 630, 668, 736, 747, 802, 843, 853, 858, 901, 935, 955, 955, 1031, 1039, 1057, 1083, 1101, 1156, 1171, 1195
		11	257, 287, 353, 572, 637, 668, 689, 696, 747, 751, 778, 793, 808, 832, 866, 918, 959, 972, 998, 1037, 1054, 1068, 1092, 1112, 1148, 1189
		12	48, 324, 341, 438, 460, 555, 561, 601, 653, 659, 671, 699, 745, 745, 761, 812, 847, 878, 892, 896, 913, 955, 1002, 1016, 1066, 1134
		13	369, 373, 397, 450, 503, 600, 737, 779, 783, 810, 879, 911, 934, 965, 988, 1000, 1009, 1018, 1046, 1056, 1084, 1115, 1152, 1188, 1240, 1263
		14	193, 259, 377, 380, 443, 492, 592, 742, 784, 795, 872, 895, 935, 970, 977, 984, 1001, 1009, 1026, 1064, 1095, 1115, 1161, 1180, 1235, 1269

		15	270, 343, 355, 387, 482, 499, 606, 624, 767, 778, 841, 891, 949, 954, 969, 978, 1008, 1016, 1069, 1077, 1087, 1120, 1152, 1213, 1246, 1270
		16	324, 336, 386, 423, 483, 500, 749, 767, 783, 802, 856, 899, 919, 946, 964, 987, 1000, 1012, 1022, 1040, 1074, 1113, 1225, 1261, 1304, 1607
Au(211)	0.22	1	291, 321, 789, 1693, 1909
	1.00	1	271, 395, 432, 486, 526, 596, 630, 694, 731, 758, 781, 852, 860, 903, 962, 968, 984, 1075, 1091, 1104, 1144, 1158, 1229, 1251, 1363, 1907
		2	374, 407, 419, 454, 561, 598, 648, 658, 684, 737, 747, 804, 877, 894, 920, 987, 1039, 1048, 1085, 1101, 1150, 1175, 1216, 1227, 1242, 1265
		3	375, 451, 484, 517, 567, 591, 611, 645, 690, 725, 764, 809, 844, 890, 899, 931, 947, 978, 987, 1055, 1146, 1195, 1251, 1283, 1372, 1805
		4	343, 410, 458, 488, 517, 557, 566, 588, 611, 644, 738, 819, 837, 879, 905, 922, 961, 989, 1025, 1098, 1129, 1216, 1274, 1384, 1396, 1740
		5	312, 398, 409, 430, 436, 465, 516, 530, 591, 675, 778, 891, 952, 972, 979, 1010, 1064, 1083, 1105, 1131, 1168, 1215, 1231, 1240, 1347, 1810
		6	328, 365, 387, 405, 467, 475, 491, 610, 626, 677, 784, 804, 821, 849, 878, 900, 960, 987, 1042, 1055, 1126, 1130, 1196, 1213, 1243, 1805
		7	245, 363, 401, 450, 508, 523, 553, 608, 691, 722, 749, 759, 781, 802, 830, 846, 888, 914, 937, 988, 1024, 1045, 1140, 1172, 1193, 1850
		8	318, 342, 400, 418, 459, 518, 592, 669, 681, 699, 739, 741, 791, 806, 830, 859, 890, 933, 948, 960, 974, 1014, 1062, 1144, 1253, 1488
Cu(211)	0.22	1	241, 546, 659, 1604, 1647
	1.00	1	423, 513, 569, 606, 671, 704, 707, 727, 796, 828, 903, 938, 974, 1003, 1015, 1021, 1042, 1055, 1093, 1103, 1111, 1157, 1164, 1200, 1238, 1268
		2	286, 408, 445, 608, 695, 709, 787, 789, 886, 908, 937, 950, 987, 1003, 1028, 1054, 1079, 1081, 1082, 1101, 1120, 1131, 1136, 1164, 1180, 1287
		3	316, 404, 472, 635, 648, 704, 742, 778, 817, 839, 883, 887, 921, 944, 993, 1036, 1075, 1098, 1104, 1136, 1161, 1174, 1205, 1230, 1285, 1311
		4	333, 391, 421, 552, 655, 766, 890, 908, 952, 991, 1002, 1005, 1009, 1012, 1014, 1033, 1053, 1056, 1079, 1096, 1125, 1137, 1154, 1174, 1610, 1751
		5	228, 328, 419, 506, 516, 662, 709, 747, 759, 821, 878, 899, 911, 924, 960, 995, 1047, 1051, 1067, 1088, 1118, 1142, 1156, 1161, 1508, 1746
		6	198, 340, 375, 394, 424, 538, 594, 728, 738, 742, 829, 845, 891, 907, 932, 971, 1006, 1013, 1061, 1092, 1141, 1177, 1188, 1302, 1483, 1596
		7	406, 417, 436, 730, 829, 855, 904, 944, 952, 988, 996, 1031, 1046, 1051, 1063, 1076, 1093, 1101, 1141, 1162, 1163, 1182, 1262, 1283, 1284, 1307
		8	363, 407, 441, 812, 850, 878, 912, 977, 991, 993, 1003, 1018, 1044, 1052, 1081, 1094, 1111, 1152, 1156, 1164, 1183, 1203, 1245, 1283, 1313, 1385
		9	274, 410, 427, 448, 716, 767, 896, 935, 981, 995, 1039, 1053, 1060, 1087, 1096, 1113, 1150, 1162, 1166, 1204, 1212, 1233, 1246, 1252, 1319, 1332

	10	359, 394, 428, 526, 750, 886, 909, 976, 990, 995, 1007, 1025, 1042, 1078, 1086, 1091, 1103, 1113, 1150, 1166, 1202, 1223, 1252, 1318, 1335, 1359
	11	321, 400, 451, 519, 904, 937, 945, 970, 975, 987, 992, 1001, 1021, 1034, 1049, 1076, 1084, 1096, 1113, 1139, 1146, 1158, 1215, 1272, 1538, 1757
	12	277, 414, 439, 515, 706, 797, 842, 847, 938, 962, 1005, 1039, 1068, 1074, 1104, 1124, 1140, 1164, 1192, 1213, 1236, 1243, 1283, 1286, 1303, 1319
	13	270, 405, 436, 469, 718, 800, 859, 889, 917, 988, 991, 1042, 1054, 1058, 1089, 1110, 1118, 1126, 1169, 1203, 1212, 1228, 1264, 1269, 1291, 1308
	14	371, 430, 466, 497, 576, 679, 799, 904, 924, 978, 1027, 1050, 1058, 1100, 1104, 1118, 1143, 1153, 1172, 1202, 1251, 1285, 1310, 1313, 1343, 1408
	15	293, 363, 447, 497, 560, 587, 692, 906, 951, 987, 1010, 1034, 1048, 1089, 1106, 1134, 1159, 1166, 1184, 1202, 1228, 1287, 1315, 1324, 1433, 1722
	16	316, 345, 434, 468, 553, 605, 621, 800, 904, 917, 997, 1036, 1069, 1100, 1134, 1153, 1158, 1179, 1189, 1212, 1218, 1251, 1281, 1305, 1333, 1387