

Supporting information to: Diffusion of Al, O, Pt, Hf, and Y atoms on α - $\text{Al}_2\text{O}_3(0001)$: Implications for the role of alloying elements in thermal barrier coatings

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Calculated vibrational frequencies

Here, we provide a list of the calculated vibrational frequencies that have been used to calculate diffusion rates using Equations 9 and 10 in the original manuscript. For the heavy adsorbates Pt, Hf and Y, only the adsorbate itself is displaced and therefore, three frequencies are obtained. For the light adsorbates Al and O, also atoms in the vicinity are displaced. For Al and O, we include all atoms within a 5 Å radius of the transition state.

Diffusion of Al

Vibrational frequencies of initial state Al4 (in cm^{-1})

806, 764, 692, 684, 676, 644, 604, 591, 561, 526, 516, 515, 510, 485, 448, 437, 428, 406, 382, 364, 354, 347, 339, 315, 282, 248, 223, 221, 199, 180

Vibrational frequencies of TS (in cm^{-1})

814, 800, 755, 746, 675, 640, 622, 590, 583, 571, 545, 522, 493, 476, 457, 421, 417, 380, 363, 356, 349, 329, 297, 283, 272, 235, 180, 153, 133, 39i

Diffusion of O

Vibrational frequencies of initial state O2 (in cm^{-1})

927, 919, 905, 897, 883, 857, 841, 804, 780, 756, 703, 686, 681, 668, 655, 654, 642, 629, 627, 622, 618, 609, 600, 593, 587, 584, 582, 564, 563, 549, 538, 534, 528, 521, 517, 514, 512, 506, 498, 484, 477, 474, 466, 462, 453, 450, 441, 437, 430, 429, 424, 413, 407, 388, 380, 371, 362, 352, 343, 337, 335, 319, 313, 303, 293, 284, 273, 258, 254, 248, 237, 222, 217, 201, 188, 185, 178, 170

Vibrational frequencies of TS1 (in cm^{-1})

1849, 919, 890, 873, 858, 845, 823, 774, 747, 732, 722, 705, 679, 668, 666, 657, 646, 635, 631, 626, 614, 607, 600, 593, 588, 579, 565, 560, 551, 548, 544, 533, 521, 510, 508, 495, 492, 490, 479, 472, 471, 466, 463, 456, 454, 450, 441, 431, 427, 414, 409, 402, 396, 390, 376, 371, 349, 344, 340, 328, 323, 315, 312, 303, 291, 279, 279, 265, 252, 244, 231, 224, 212, 198, 183, 155, 121, 1810i

Vibrational frequencies of intermediate state O5 (in cm⁻¹)

926, 915, 898, 891, 858, 853, 800, 773, 752, 738, 728, 703, 679, 673, 662, 646, 644, 636, 629, 624, 620, 610, 600, 598, 588, 583, 577, 564, 554, 550, 546, 535, 520, 515, 511, 505, 504, 500, 489, 478, 474, 467, 464, 461, 452, 447, 440, 438, 431, 419, 414, 410, 400, 388, 383, 369, 356, 353, 346, 336, 329, 324, 316, 314, 302, 294, 276, 266, 265, 260, 246, 236, 219, 214, 191, 187, 184, 163

Vibrational frequencies of TS2 (in cm⁻¹)

925, 919, 903, 874, 855, 845, 816, 777, 751, 742, 724, 705, 696, 678, 670, 654, 646, 636, 630, 625, 617, 611, 603, 596, 588, 582, 574, 570, 565, 555, 545, 539, 536, 520, 514, 509, 507, 500, 487, 482, 472, 466, 460, 457, 452, 448, 437, 434, 429, 425, 406, 398, 392, 384, 373, 359, 349, 347, 338, 331, 325, 321, 315, 309, 298, 290, 280, 256, 252, 248, 240, 222, 211, 207, 190, 183, 163, 163i

Diffusion of Pt

Vibrational frequencies of initial state O2 (in cm⁻¹)

111, 61, 25

Vibrational frequencies of TS1 (in cm⁻¹)

126, 27, 22i

Vibrational frequencies of intermediate state O5 (in cm⁻¹)

100, 55, 8

Vibrational frequencies of TS2 (in cm⁻¹)

105, 57, 21i

Diffusion of Hf

Vibrational frequencies of initial state Al4 (in cm⁻¹)

125, 105, 92

Vibrational frequencies of TS (in cm⁻¹)

135, 102, 28i

Vibrational frequencies of intermediate state Al3 (in cm⁻¹)

136, 96, 88

Diffusion of Y

Vibrational frequencies of initial state Al4 (in cm⁻¹)

178, 126, 121

Vibrational frequencies of TS (in cm⁻¹)

237, 169, 43i

Vibrational frequencies of intermediate state AI3 (in cm⁻¹)

174, 119, 116