**W(100) surface definitions**

**Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_other:w100_definition.pdf**

**Numerical data tables for lowest-energy configurations examines on the W(100) surface (high convergence numbers)**

The values presented in the table below were calculated using the PBE XC functional with the corresponding Vanderbilt USPPs for W and H, 260 bands (10 bands/W atom), and energy cutoffs of 40 Ry and 320 Ry for the wave-function and electron density, respectively. Total electronic energy was considered self-consistent at a threshold of 1.0 x 10^-9 Ry. Atomic coordinates were optimized to a force threshold of 1 x 10^-7 eV/A; subsequently phonons were calculated using DFT-PT holding all W atoms fixed in space until the forces were self-consistent to a threshold of 1.4 x 10^-12 eV/A.

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| **W(100)** | | | | | |
| Θ |  |  |  |  |  |
| 0.25 | -0.88 | -0.83 | -0.83 (ref.) | -0.83 | 0.00 (ref.) |
| 0.5 | -1.79 | -1.69 | -0.86 | -0.86 | -0.03 |
| 0.75 | -2.38 | -2.21 | -0.52 | -0.74 | 0.12 |
| 1.0 | -3.10 | -2.86 | -0.65 | -0.72 | 0.02 |
| 1.25 | -3.85 | -3.58 | -0.72 | -0.72 | 0.00 |
| 1.5 | -4.51 | -4.19 | -0.61 | -0.70 | 0.02 |
| 1.75 | -5.23 | -4.84 | -0.65 | -0.69 | 0.01 |
| 2.0 | -5.98 | -5.49 | -0.65 | -0.69 | 0.00 |
| 2.25 | -6.00 | -5.59 | -0.10 | -0.62 | 0.07 |
| 2.5 | -5.94 | -5.63 | -0.04 | -0.56 | 0.06 |
| 2.75 | -5.96 | -5.67 | -0.04 | -0.52 | 0.04 |
| 3.0 | -5.95 | -5.71 | -0.04 | -0.48 | 0.04 |

**W(100) Coverage specific data tables**

The values presented in the table below were calculated using:

PBE XC functional with Vanderbilt USPPs for W and H

208 bands

energy cutoffs of 40 Ry and 320 Ry for the wave-function and electron density

Total electronic energy was considered self-consistent at a threshold of 1.0 x 10^-7 Ry

Atomic coordinates were optimized to a force threshold of 1 x 10^-5 eV/A; subsequently phonons were calculated using DFT-PT holding all W atoms fixed in space until the forces were self-consistent to a threshold of 1.4 x 10^-10 eV/A.

Values in (parenthesis) were calculated with higher convergence modifications:

260 bands

total electronic energy was considered self-consistent at a threshold of 1.0 x 10^-9 Ry.

Atomic coordinates were optimized to a force threshold of 1 x 10^-7 eV/A

phonons were calculated using DFT-PT holding all W atoms fixed in space until the forces were self-consistent to a threshold of 1.4 x 10^-12 eV/A.

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| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv0p25_sb.eps  w100\_1H\_sb | -0.86  (-0.88) | (-0.83) | (-0.83) |  |  |

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| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv0p5_2sbA.eps  w100\_2H\_2sbA | -1.78  (-1.79) | (-1.69) | (-0.86) |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv0p5_2sbC.eps  w100\_2H\_2sbC | -1.62  (-1.63) | (-1.54) | (-0.77) |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv0p5_2sbB.eps  w100\_2H\_2sbB | -1.35 |  |  |  |  |

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| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv0p75_3sbA.eps  w100\_3H\_3sbA | -2.38  (-2.38) | (-2.21) | (-0.74) |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv0p75_3sbB.eps  w100\_3H\_3sbB | -2.22  (-2.22) | (-2.05) | (-0.69) |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv0p75_3sbC.eps  w100\_3H\_3sbC | -2.15  (X) | (X) | (X) |  |  |

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| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv1_4sbA.eps  w100\_4H\_4sbA | -3.10  (-3.10) | (-2.86) | (-0.72) |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv1_4sbB.eps  w100\_4H\_4sbB | -3.01  (-3.01) | (-2.78) | (-0.70) |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv1_4sbC.eps  w100\_4H\_4sbC | -2.97  (-2.99) | (-2.78) | (-0.70) |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv1_4sbD.eps  w100\_4H\_4sbD | -2.88  (-2.89) | (-2.72) | (-0.68) |  |  |

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| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv1p25_5sbA.eps  w100\_5H\_5sbA | -3.84  (-3.85) | (-3.58) | (-0.72) |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv1p25_5sbB.eps  w100\_5H\_5sbB | -3.72  (-3.72) | (-3.45) | (-0.69) |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv1p25_5sbC.eps  w100\_5H\_5sbC | -3.67  (-3.68) | (-3.44) | (-0.69) |  |  |

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| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv1p5_6sbA.eps  w100\_6H\_6sbA | -4.52  (-4.51) | (-4.19) | (-0.70) |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv1p5_6sbB.eps  w100\_6H\_6sbB | -4.34  (-4.44) | (-4.12) | (-0.69) |  |  |

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| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv1p75_7sbA-eps-converted-to.pdf  w100\_7H\_7sbA | -5.24  (-5.23) | (-4.84) | (-0.69) |  |  |

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| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv2_8sb.eps  w100\_8H\_8sb | -5.99  (-5.98) | (-5.49) | (-0.69) |  |  |

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| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv2p25_8sb1tf.eps  w100\_9H\_8sb1tf | -6.01  (-6.00) | (-5.59) | (-0.62) |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv2p25_8sb1top.eps  w100\_9H\_8sb1top | -5.87  (-5.86) | (-5.41) | (-0.60) |  |  |

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| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv2p5_8sb2tfB.eps  w100\_10H\_8sb2tfB | -5.94  (-5.94) | (-5.63) | (-0.56) |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv2p5_8sb1top1tfB.eps  w100\_10H\_8sb1top1tfB | -5.96  (-5.96) | (-5.59) | (-0.56) |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv2p5_8sb2tfA.eps  w100\_10H\_8sb2tfA | -5.88  (-5.88) | (-5.57) | (-0.56) |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv2p5_8sb1top1tfC.eps  w100\_10H\_8sb1top1tfC | -5.91  (-5.91) | (-5.55) | (-0.56) |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv2p5_8sb2topA.eps  w100\_10H\_8sb2topA | -5.79 |  |  |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv2p5_8sb2topB.eps  w100\_10H\_8sb2topB | -5.68 |  |  |  |  |

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| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv2p75_8sb1tf2topA.pdf  w100\_11H\_8sb1tf2topA | -5.94  (-5.93) | (-5.59) | (-0.51) |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv2p75_8sb2tf1topB.eps  w100\_11H\_8sb2tf1topB | -5.91  (-5.90) | (-5.63) | (-0.51) |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv2p75_8sb1tf2topA.eps  w100\_11H\_8sb1tf2topB | -5.91  (-5.90) | (-5.58) | (-0.51) |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv2p75_8sb2tf1topC.eps  w100\_11H\_8sb2tf1topC | -5.90  (-5.89) | (-5.62) | (-0.51) |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv2p75_8sb1tf2topC.eps  w100\_11H\_8sb1tf2topC | -5.82 |  |  |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv2p75_8sb3top.eps  w100\_11H\_8sb3top | -5.74 |  |  |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv2p75_8sb3tf.eps  w100\_11H\_8sb3tf | -5.70 |  |  |  |  |

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| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv3_MC0.pdf  w100\_12H\_MC4 | -5.95  (-5.95) | (-5.71) | (-0.48) |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv3_MC2.pdfw100\_12H\_MC2 | -5.88  (-5.88) | (-5.64) | (-0.47) |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv3_MC5.pdf  w100\_12H\_MC5 | -5.84  (-5.84) | (-5.58) | (-0.47) |  |  |
| Macintosh HD:Users:Zach:Dropbox:french_postdoc:paper_2:gfx_tables_100:w100_cv3_E0.pdf  w100\_12H\_MC0 | -5.82  (-5.82) | (-5.51) | (-0.46) |  |  |