

Systematic pseudopotentials from reference eigenvalue sets for DFT calculations

Additional information

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We display in the following pages those elements for which we are unable to improve the electronic dispersion in a significant manner: C, Al, Si, V, Cr, Cu, Se, Nb, and Te. Please refer to Table 2 in the main text to assess the overall improvement by means of the ratio Y_o/Y_i .

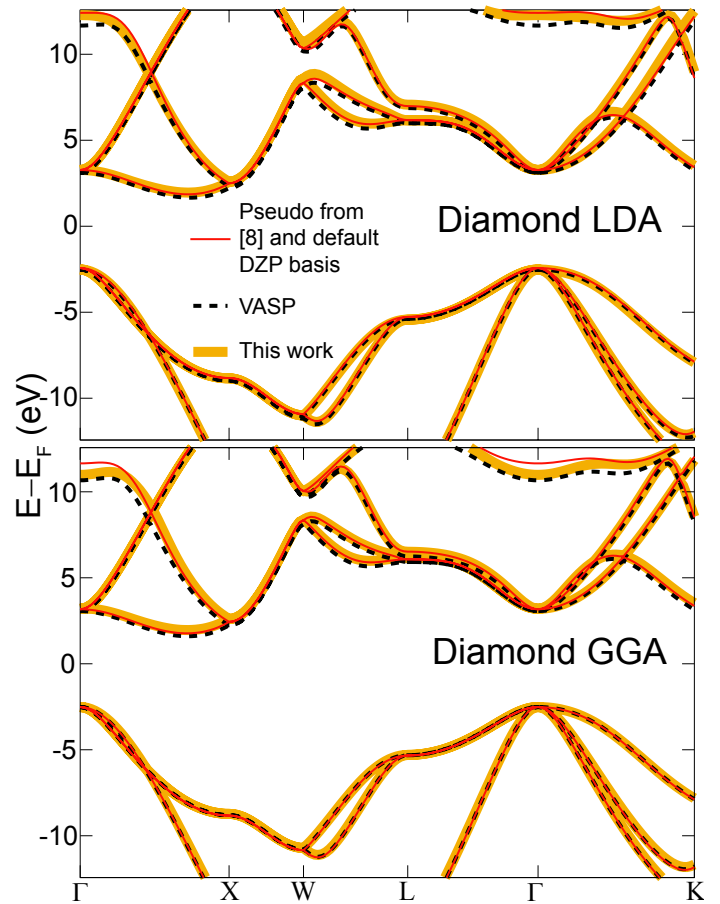


Figure 1: C (Z = 6)

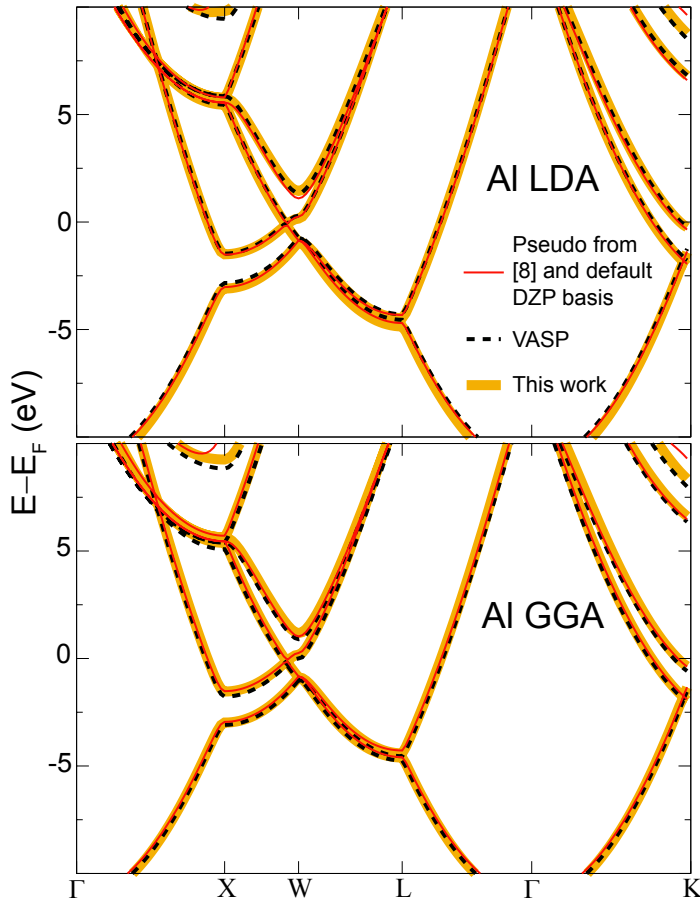


Figure 2: Al ($Z = 13$)

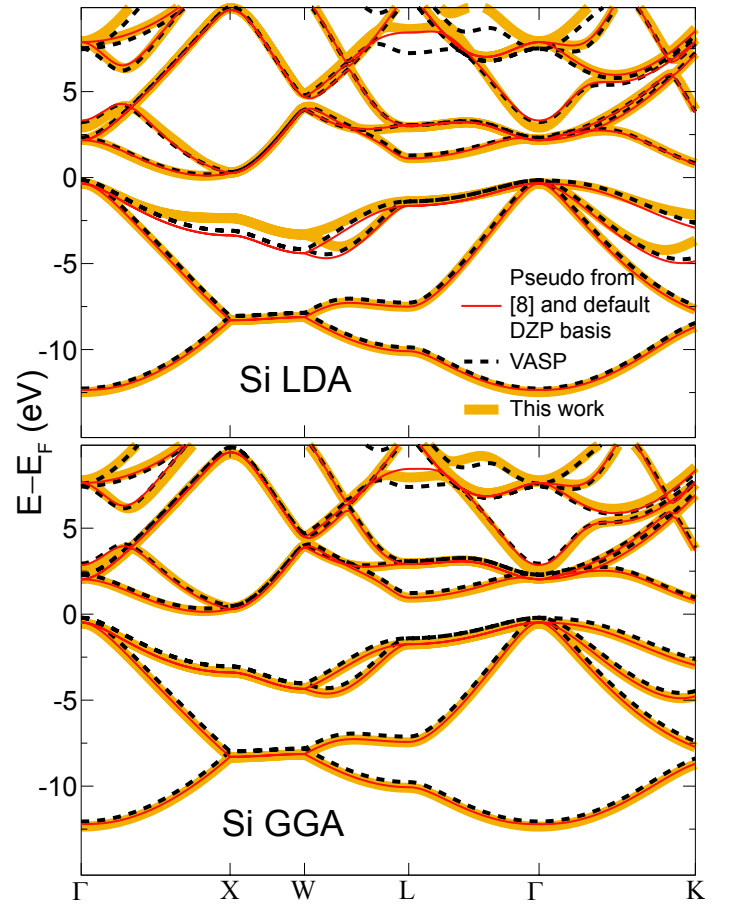


Figure 3: Si ($Z = 14$).

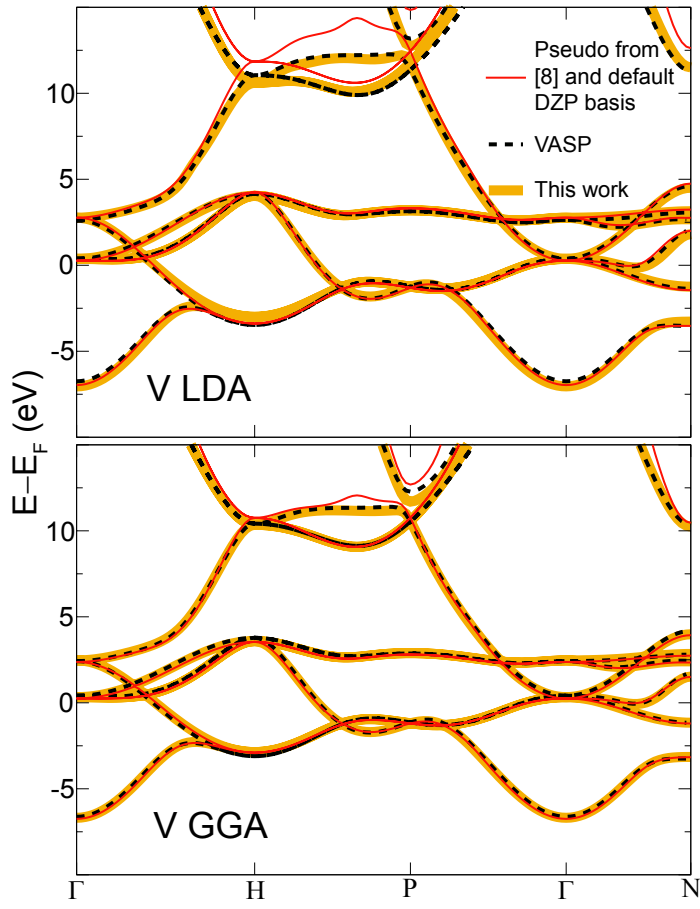


Figure 4: V ($Z = 23$).

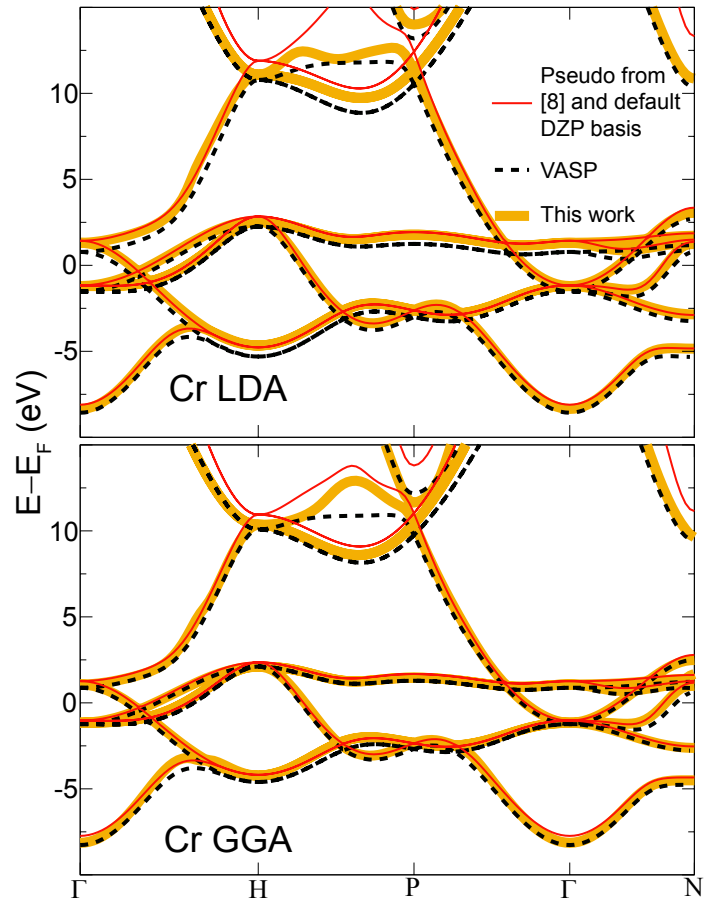


Figure 5: Cr ($Z = 24$).

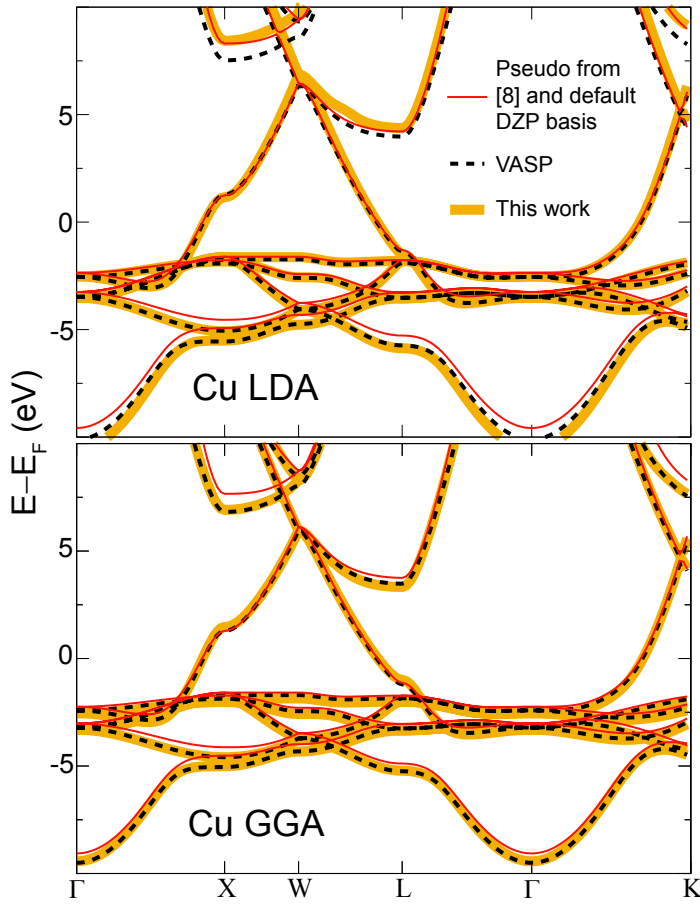


Figure 6: Cu ($Z = 29$).

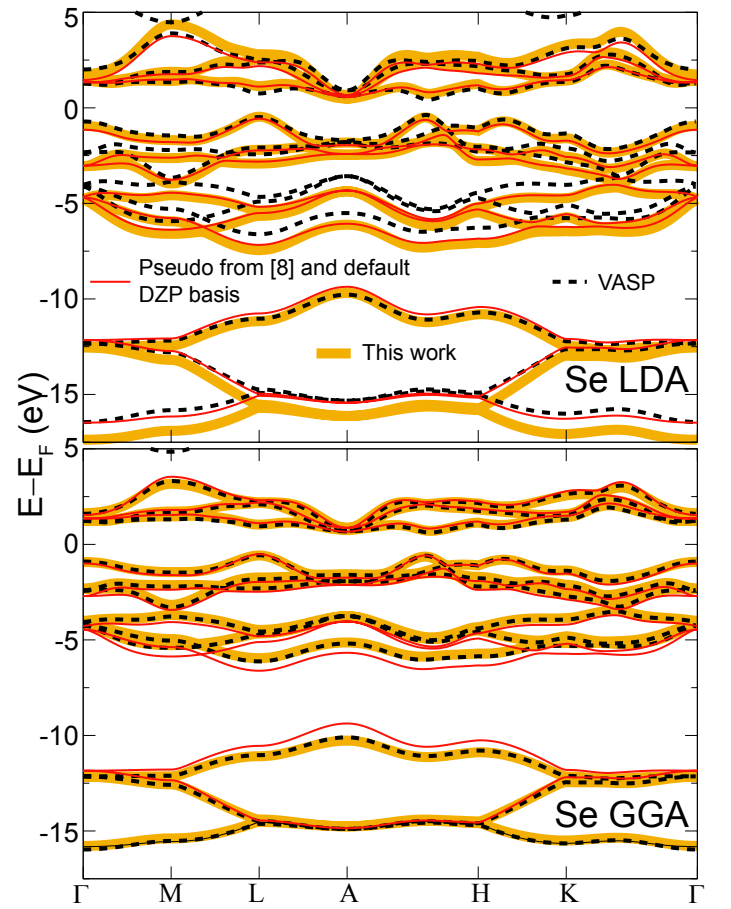


Figure 7: Se ($Z = 34$).

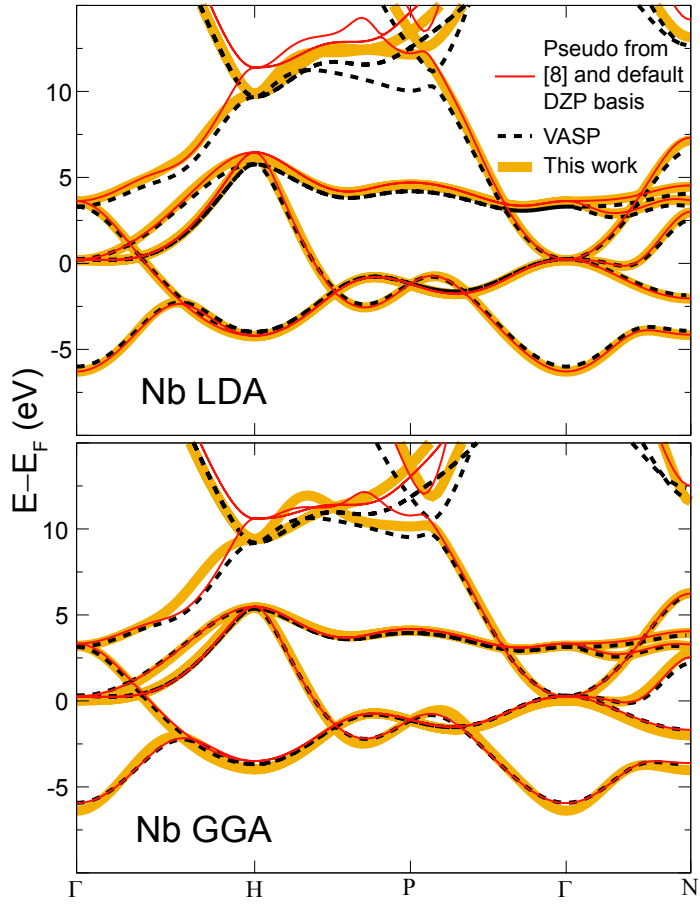


Figure 8: Nb ($Z = 41$).

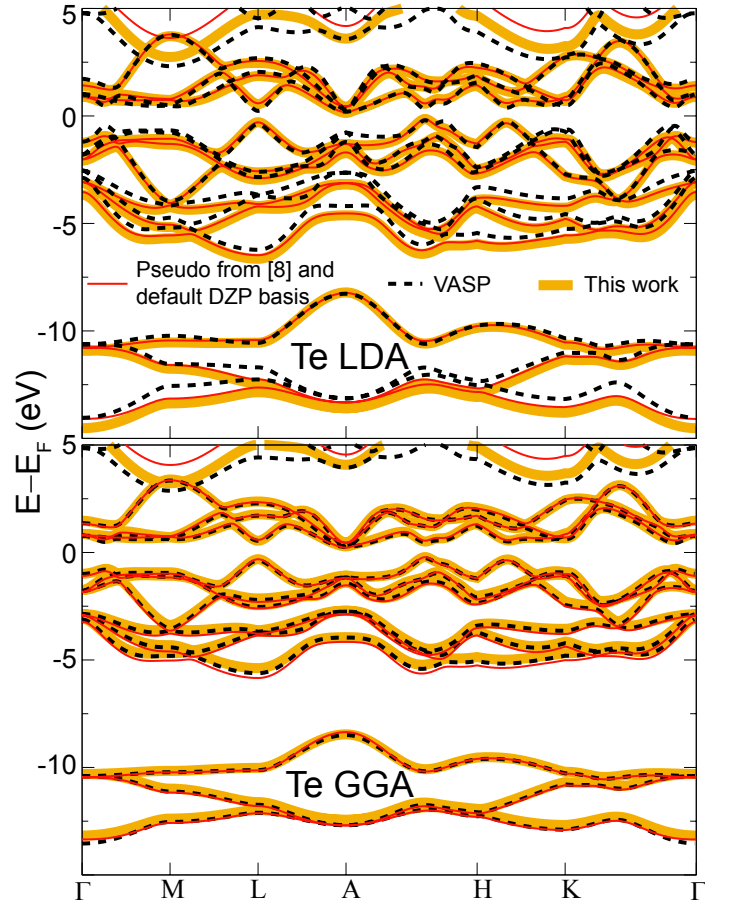


Figure 9: Te ($Z = 52$).