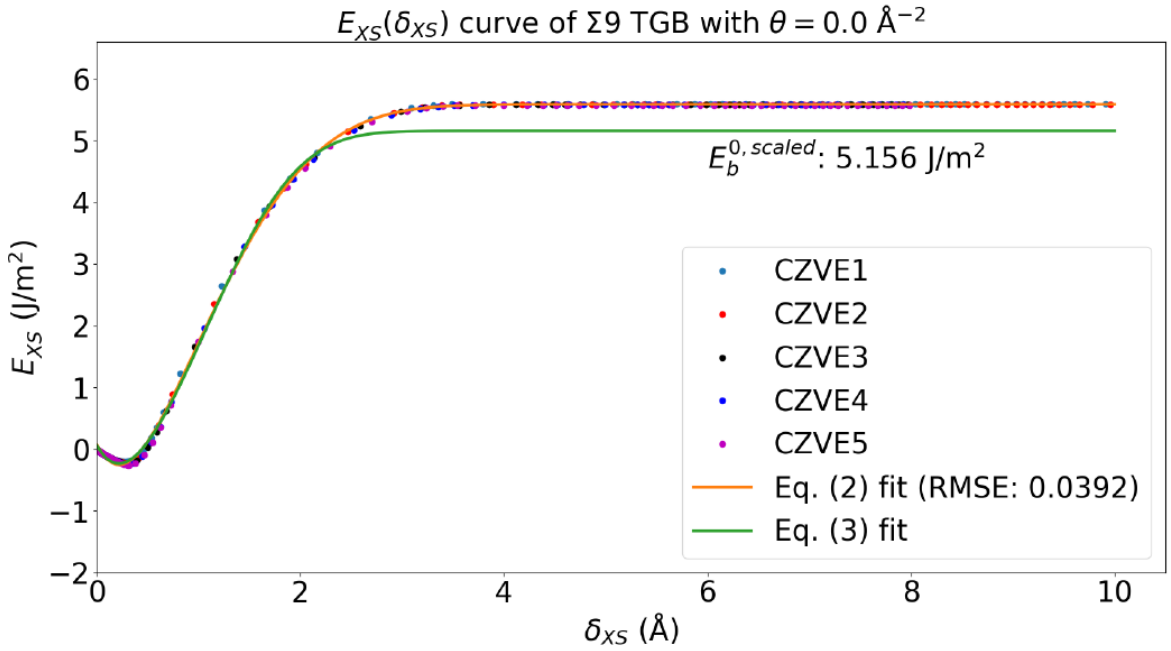
Atomistic assessment of interfacial interaction potential in tungsten twist grain boundaries: Supplementary material

S1. INTERFACIAL BINDING ENERGY.

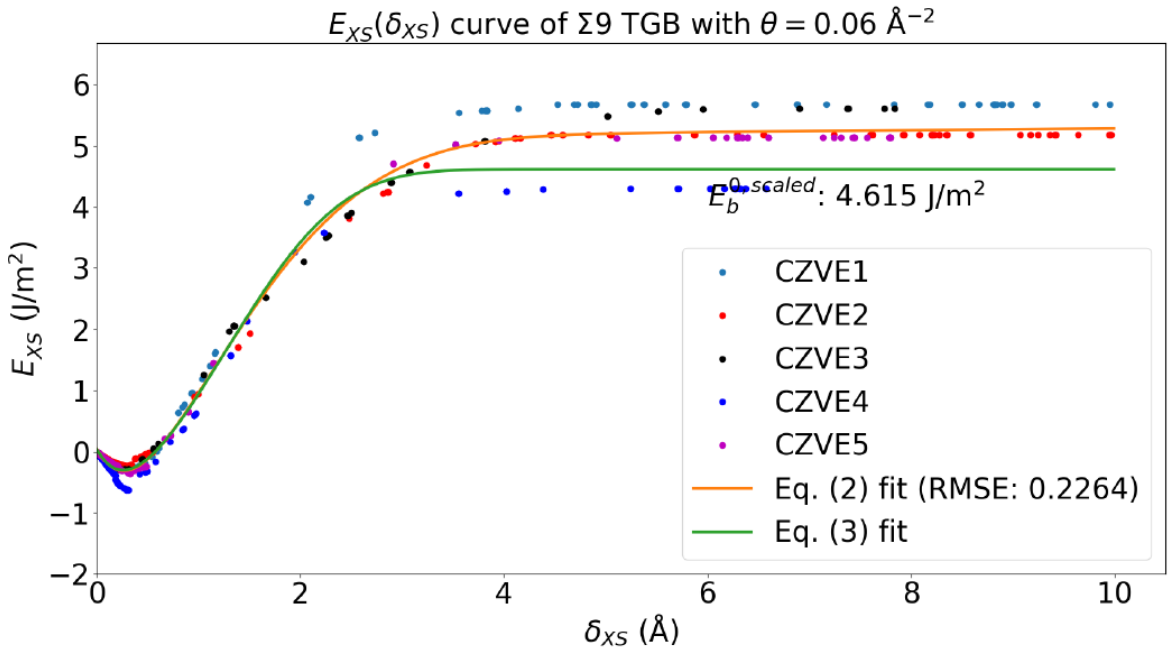
The interfacial binding energy, $E_b^{0,scaled}$, from the parameterized xUBER (Eq. (3) in the main article), for all the considered TGBs with P impurity coverage, $\theta = 0.0$ and 0.06 Å^{-2}, is provided in Table S1.

Table S1. Interfacial binding energy ($E_b^{0,scaled}$ in units of Jm^2) of the $\langle 110 \rangle$ TGBs considered in the present work. Here, θ stands for P impurities coverage and $W_{GB}^{sep} = 2\gamma_{\{110\}} - \gamma_{GB}$.

GB, crack system	$E_b^{0,scaled}$		W_{GB}^{sep}	$\frac{\lvert W_{GB}^{sep} - E_b^{0,scaled} \rvert}{W_{GB}^{sep}}$%
Σ	$\theta = 0.0$ Å^{-2}	$\theta = 0.06$ Å^{-2}	$\theta = 0.0$ Å^{-2}	$\theta = 0.0$ Å^{-2}
Σ51	5.197	4.297	5.190	$\sim$0.13
Σ33	5.156	4.657	5.146	$\sim$0.2
Σ19	5.139	4.641	5.127	$\sim$0.23
Σ27	5.225	4.804	5.104	$\sim$2.37
Σ9	5.156	4.615	5.144	$\sim$0.23
Σ11	5.252	4.569	5.220	$\sim$0.6
Σ41	5.146	4.229	5.138	$\sim$0.16
Σ3	5.914	5.233	5.890	$\sim$0.4
Σ43	5.347	4.408	5.326	$\sim$0.4
Σ17	5.263	4.854	5.252	$\sim$0.21

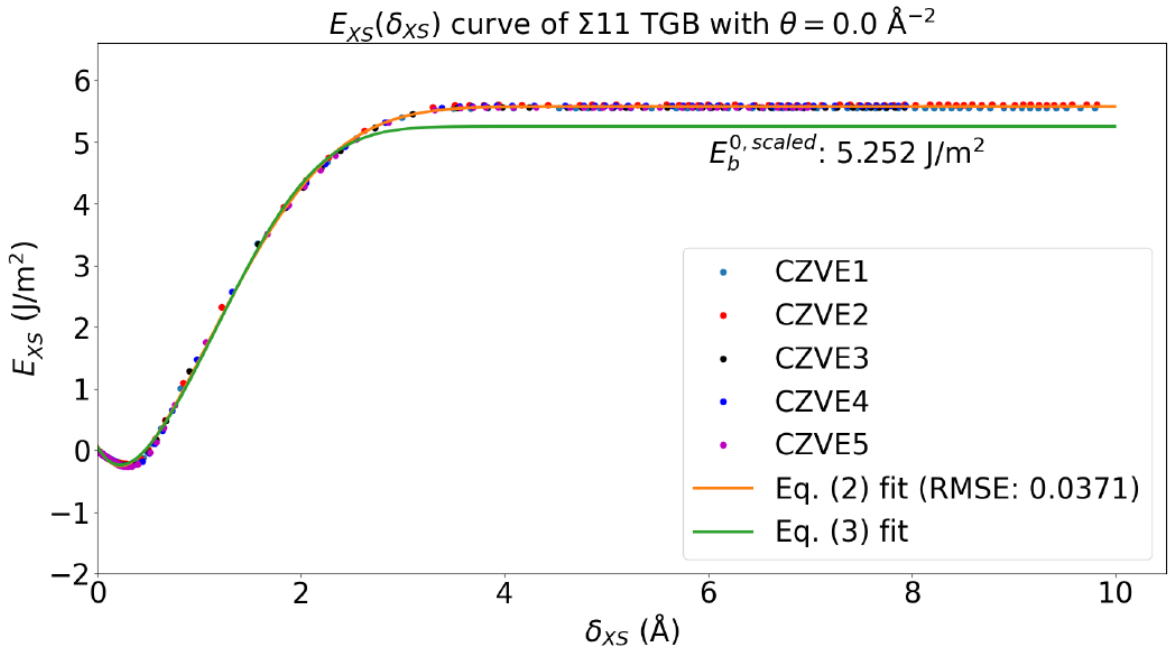


(a)

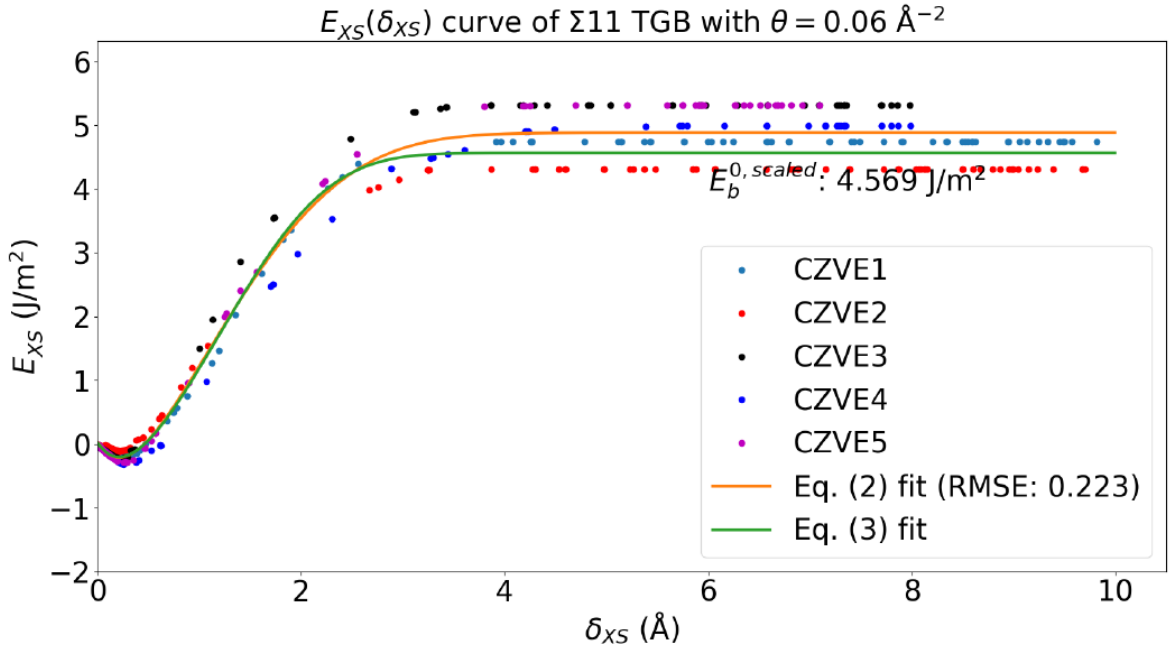


(b)

Fig. S1. Excess interface energetics ($E_{XS}(\delta_{XS})-$curve) for (a) pristine and (b) $\theta = 0.06$ Å^{-2} Σ9 TGB.

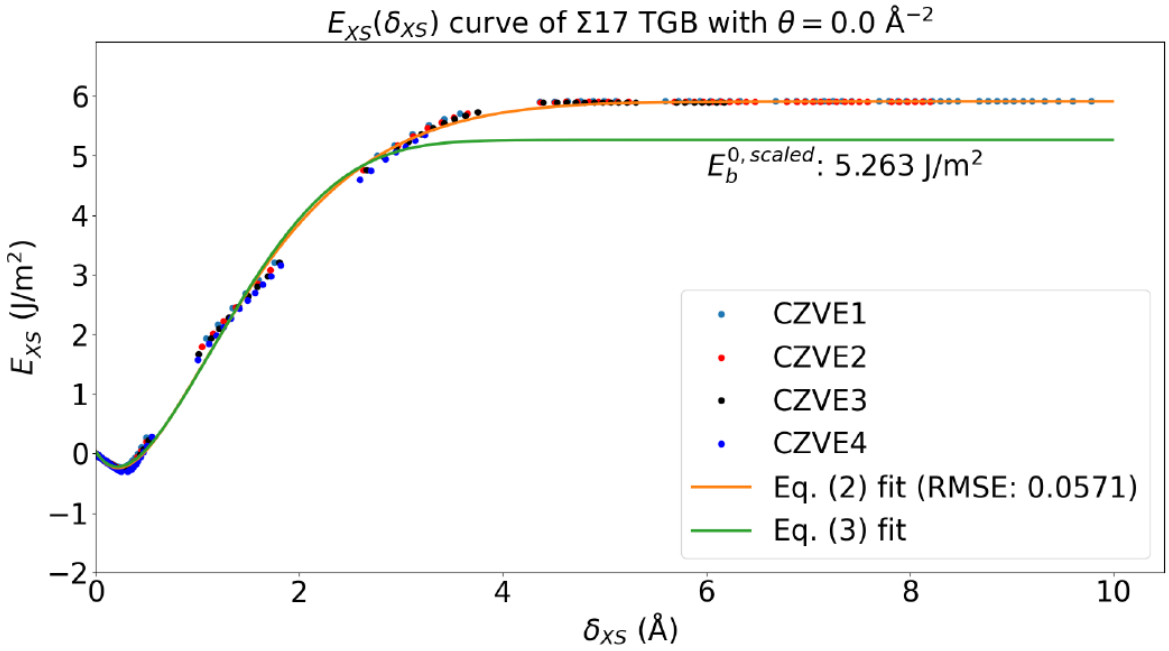


(a)

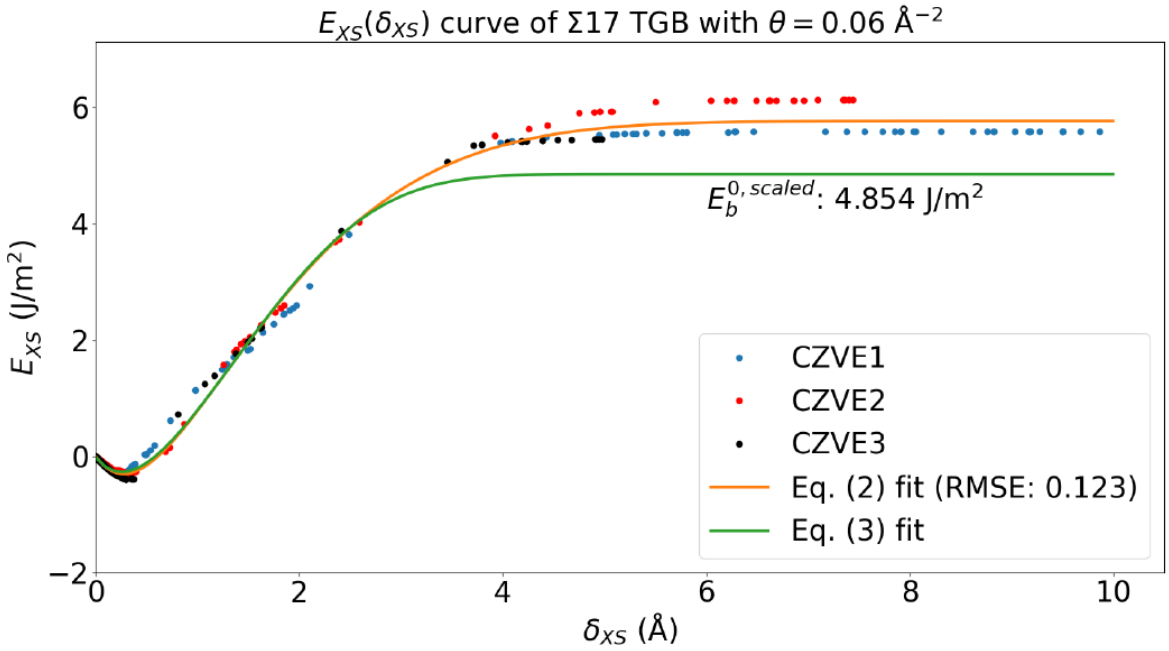


(b)

Fig. S2. Excess interface energetics ($E_{XS}(\delta_{XS})-$curve) for (a) pristine and (b) $\theta = 0.06$ Å^{-2} Σ11 TGB.

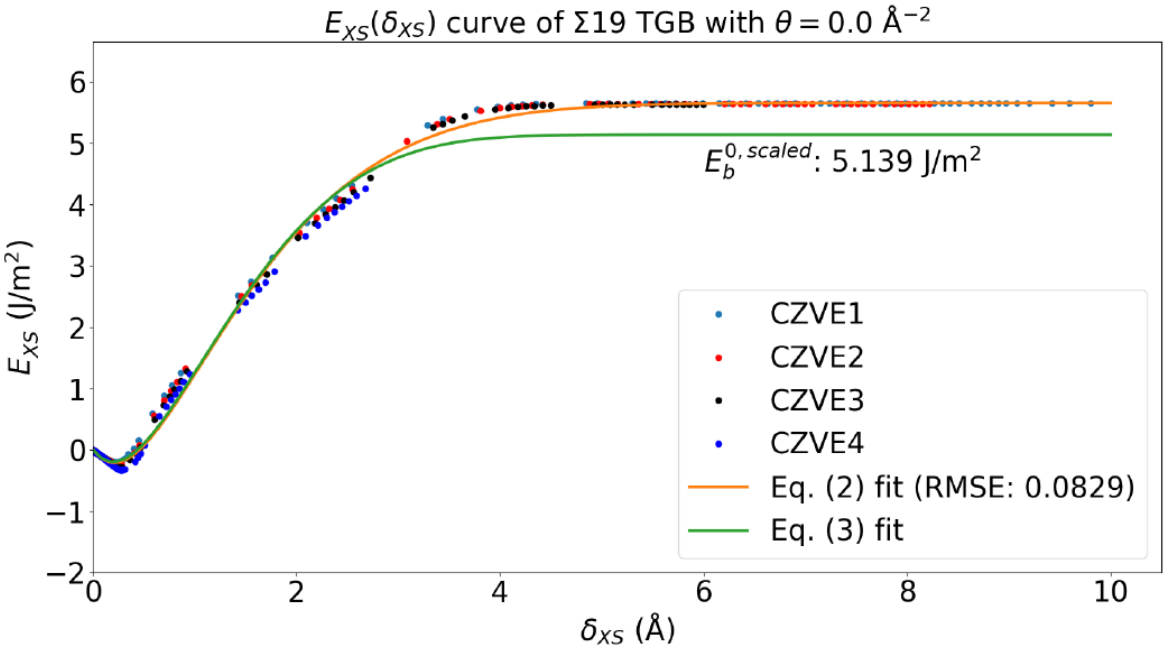


(a)

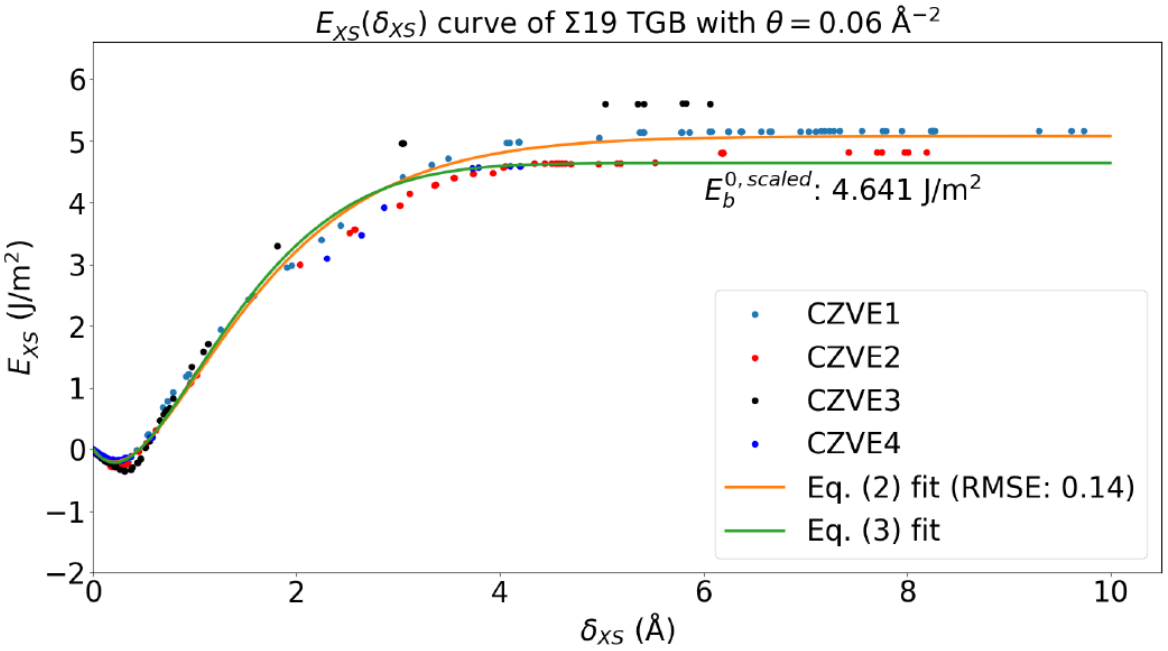


(b)

Fig. S3. Excess interface energetics ($E_{XS}(\delta_{XS})-$curve) for (a) pristine and (b) $\theta = 0.06$ Å^{-2} Σ17 TGB.

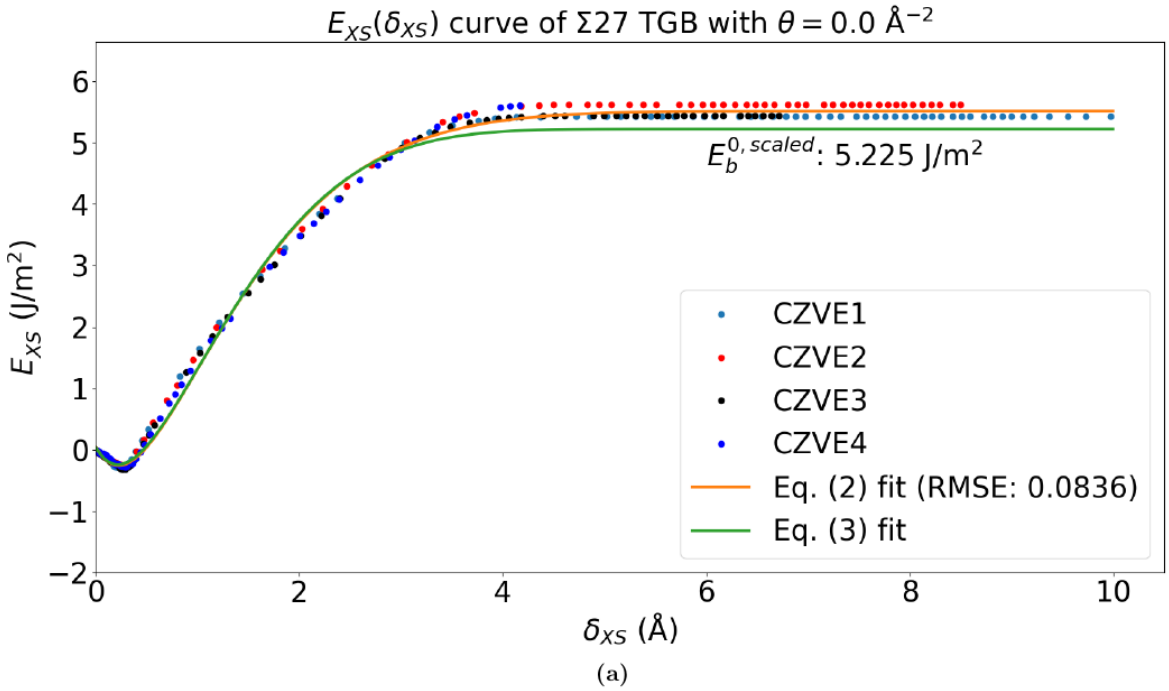


(a)

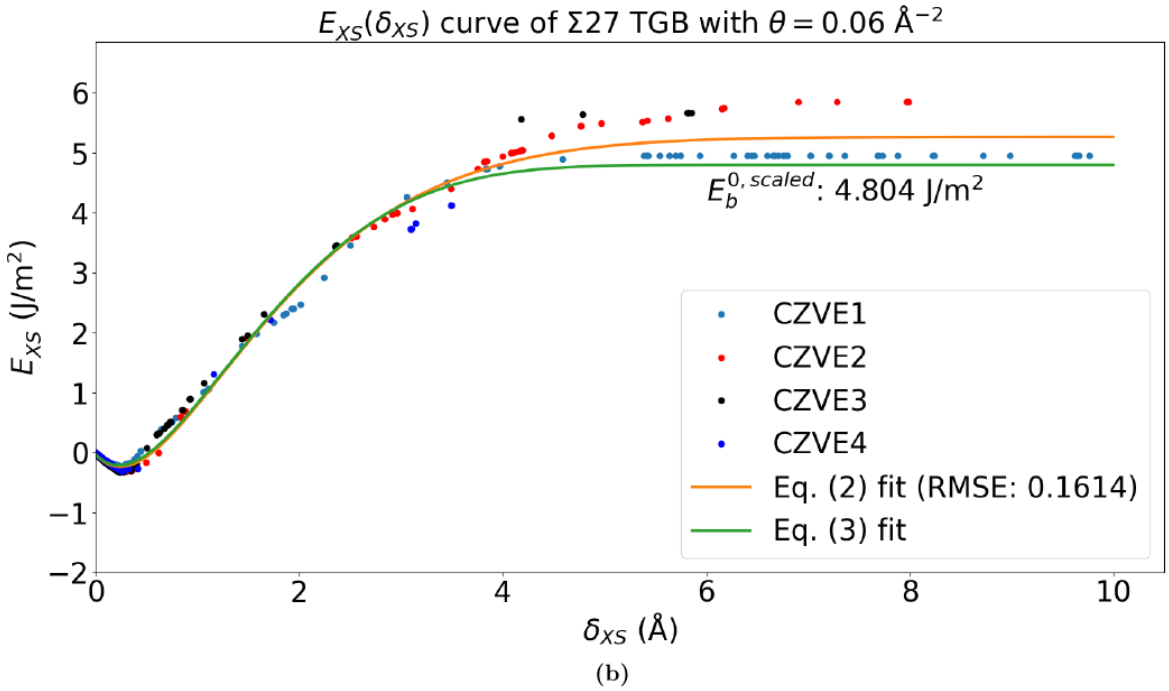


(b)

Fig. S4. Excess interface energetics ($E_{XS}(\delta_{XS})-$curve) for (a) pristine and (b) $\theta = 0.06$ Å^{-2} Σ19 TGB.

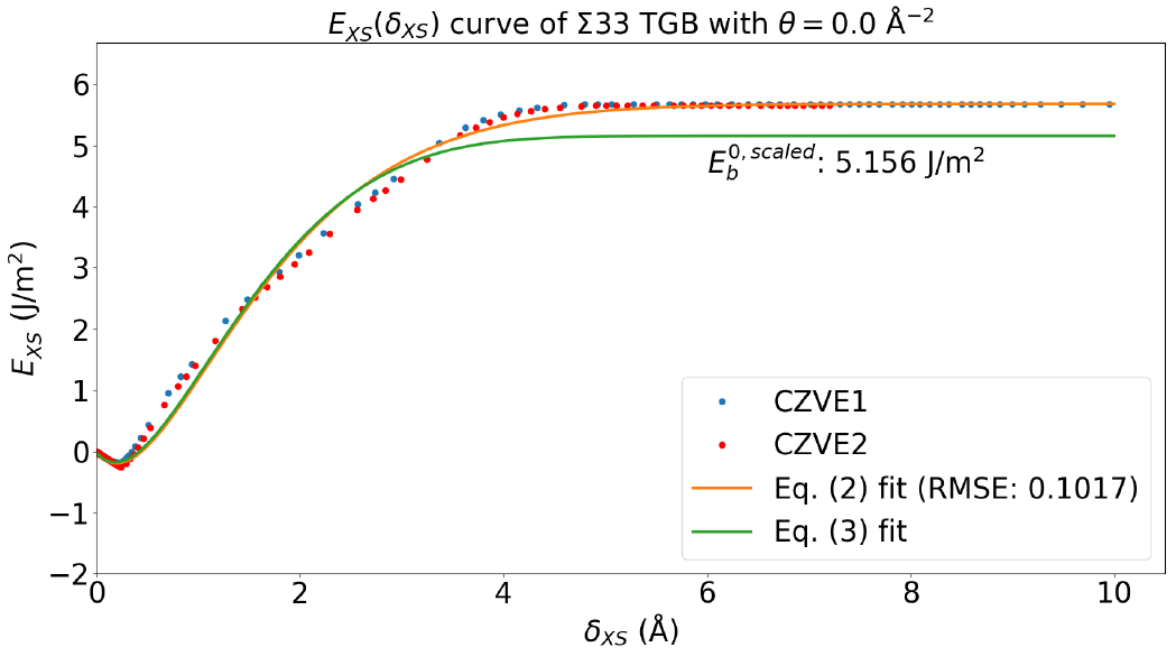


(a)

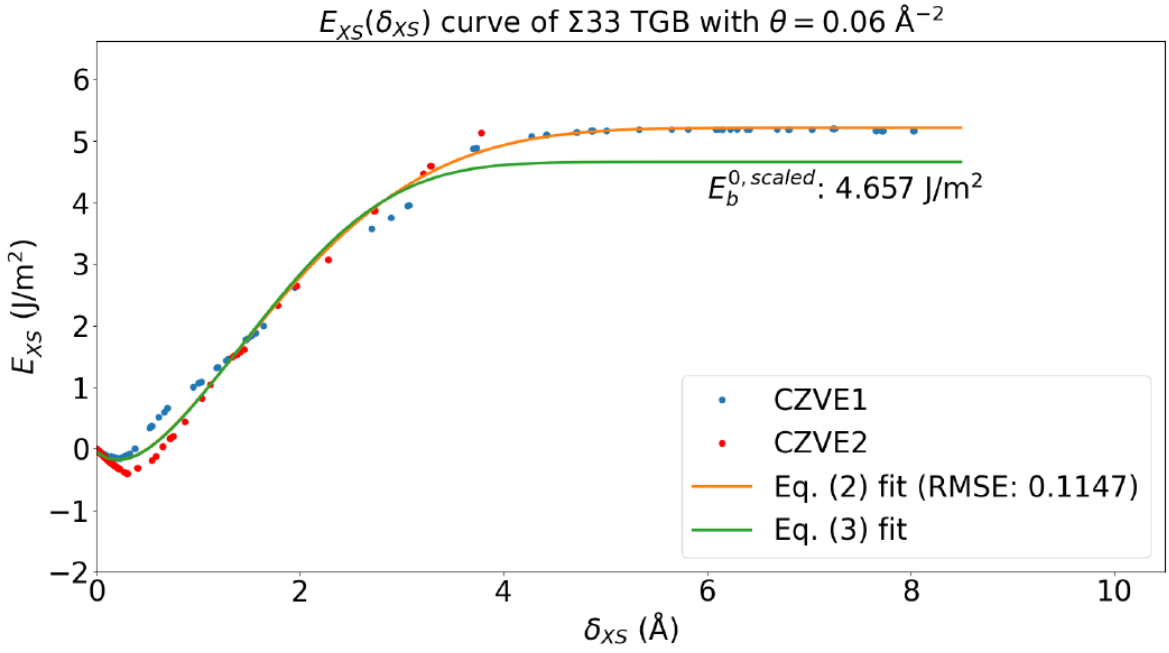


(b)

Fig. S5. Excess interface energetics ($E_{XS}(\delta_{XS})-$curve) for (a) pristine and (b) $\theta = 0.06$ Å^{-2} Σ27 TGB.

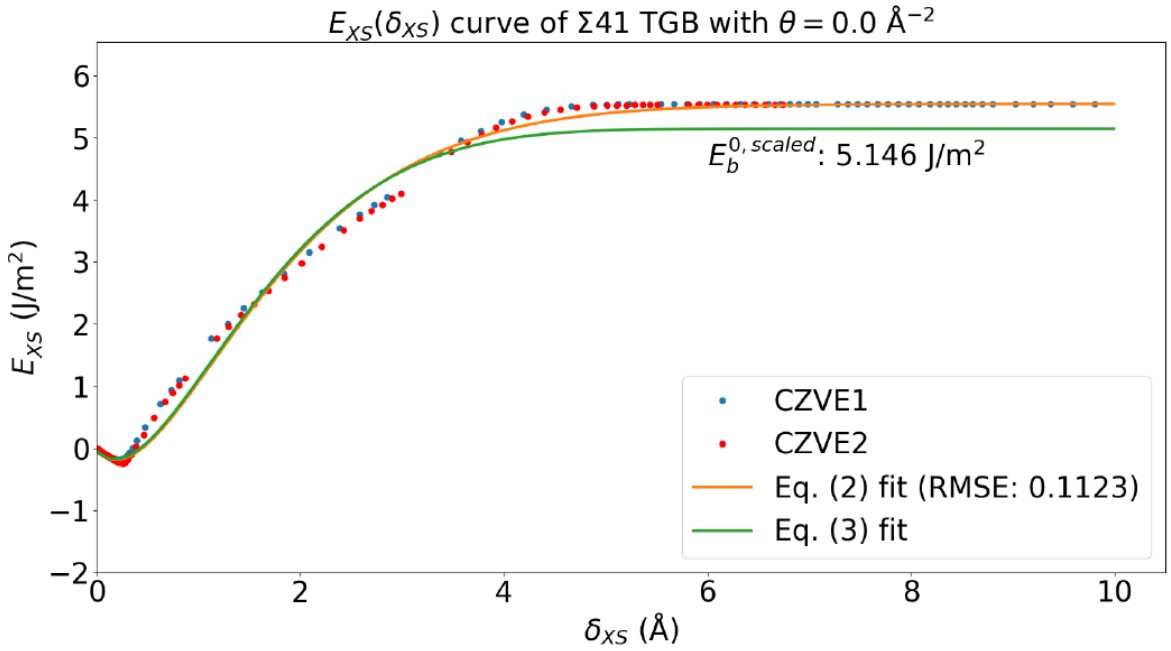


(a)

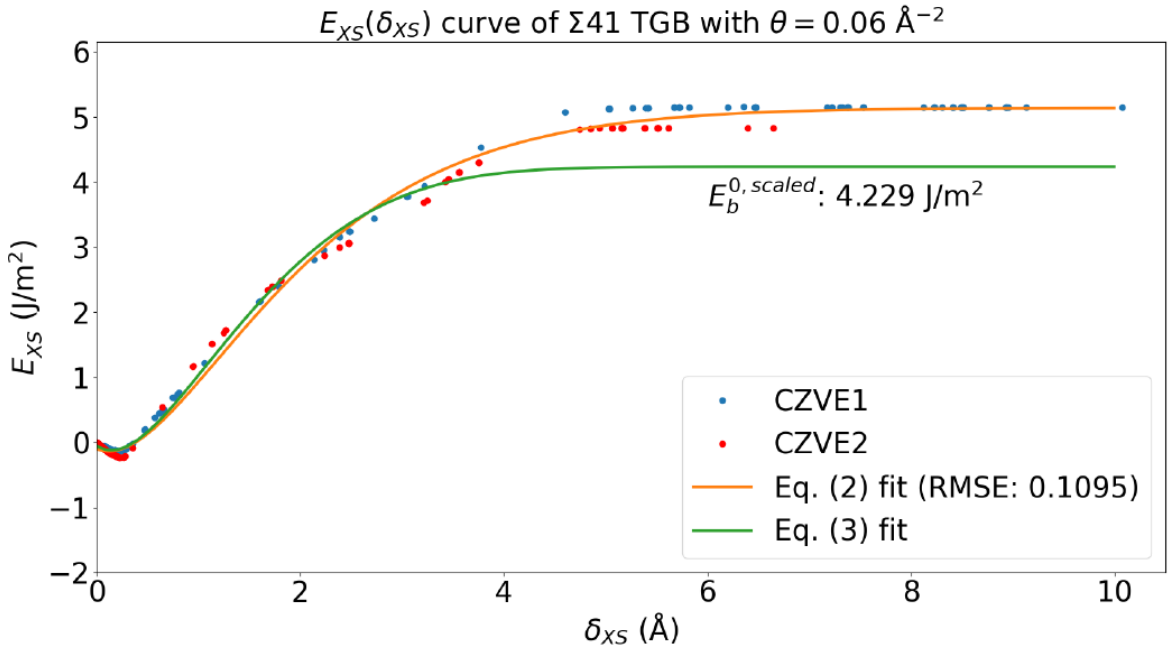


(b)

Fig. S6. Excess interface energetics ($E_{XS}(\delta_{XS})-$curve) for (a) pristine and (b) $\theta = 0.06$ Å^{-2} Σ33 TGB.

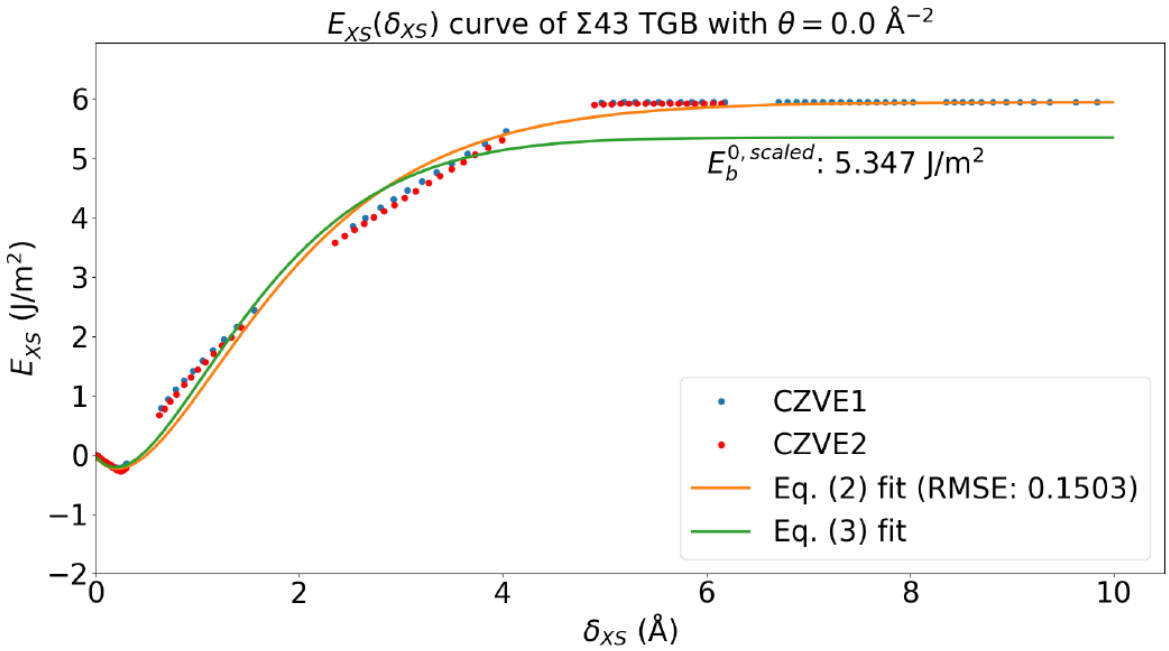


(a)

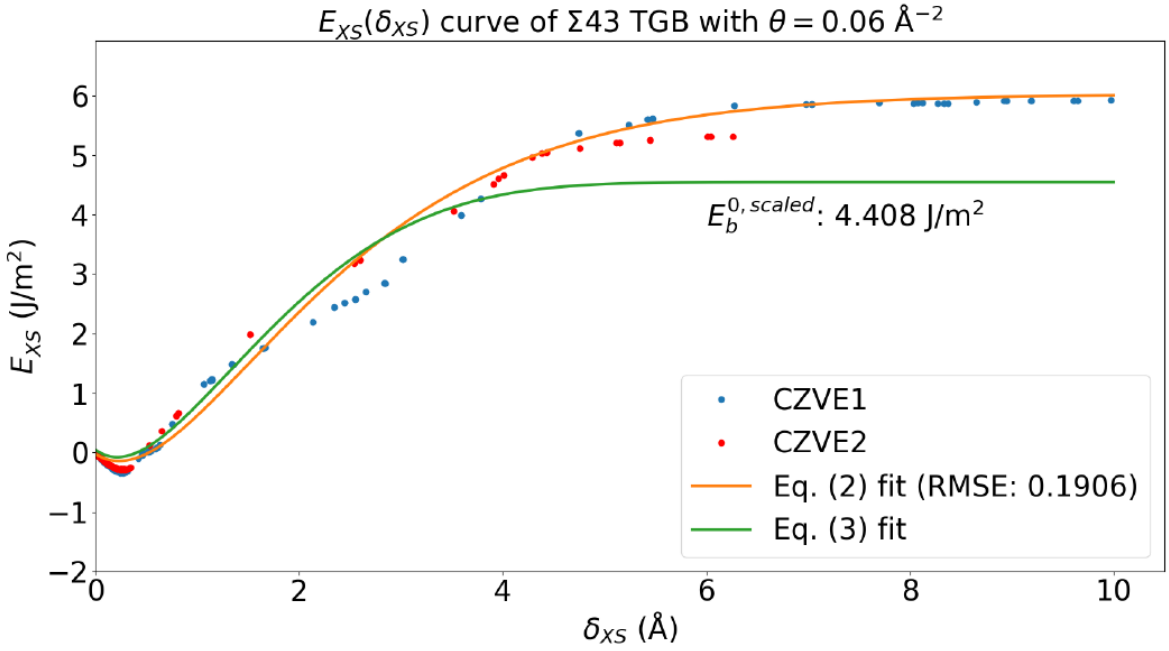


(b)

Fig. S7. Excess interface energetics ($E_{XS}(\delta_{XS})-$curve) for (a) pristine and (b) $\theta = 0.06$ Å^{-2} Σ41 TGB.

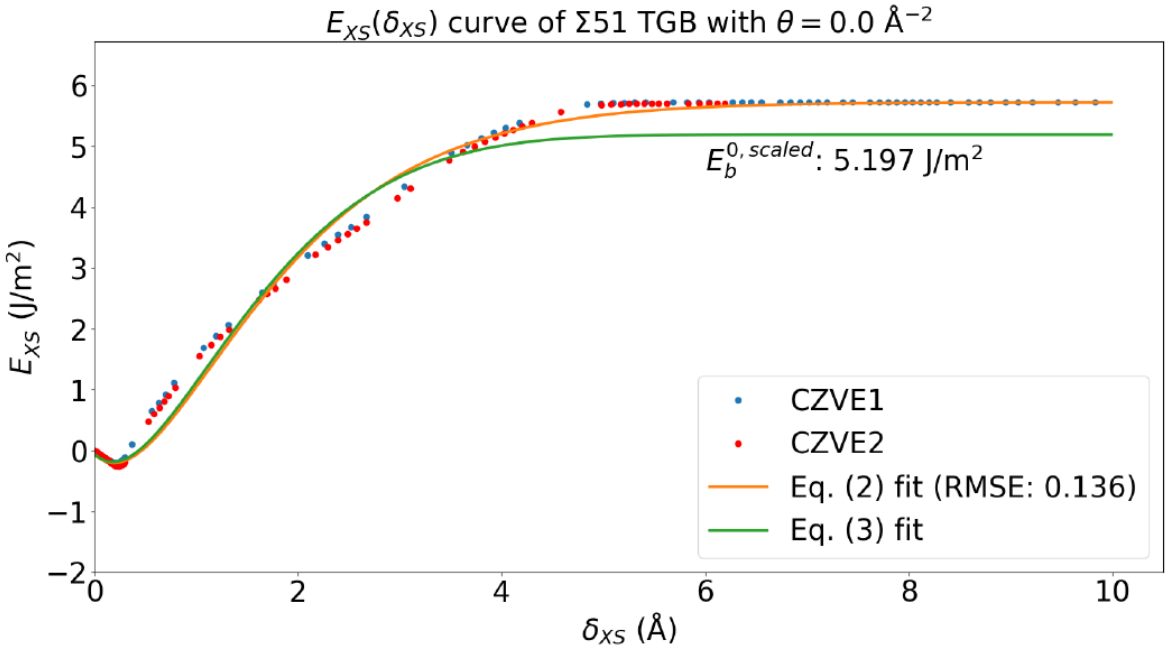


(a)

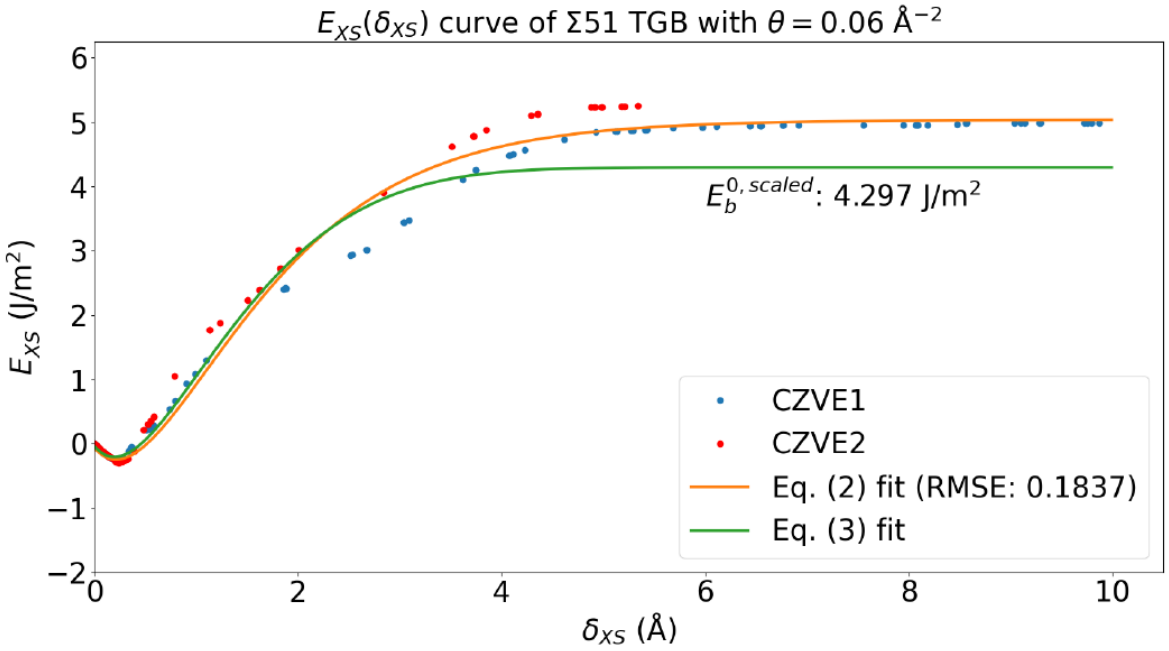


(b)

Fig. S8. Excess interface energetics ($E_{XS}(\delta_{XS})-$curve) for (a) pristine and (b) $\theta = 0.06$ Å^{-2} Σ43 TGB.



(a)



(b)

Fig. S9. Excess interface energetics ($E_{XS}(\delta_{XS})-$curve) for (a) pristine and (b) $\theta = 0.06$ Å^{-2} Σ51 TGB.

S2. TRACTION-SEPARATION CURVES AND PEAK STRESS

The traction-separation curves are given in Figures S10-S18 and the corresponding peak stresses are tabulated in Table S2.

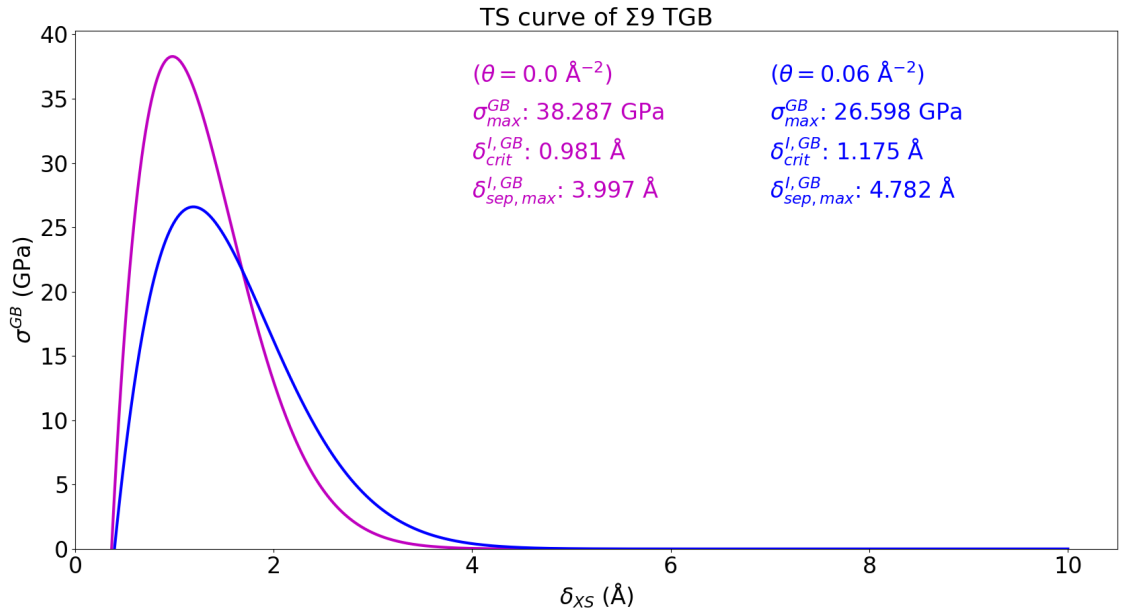


Fig. S10. TS curves for (a) pristine and (b) $\theta = 0.06$ Å^{-2} Σ9 TGB.

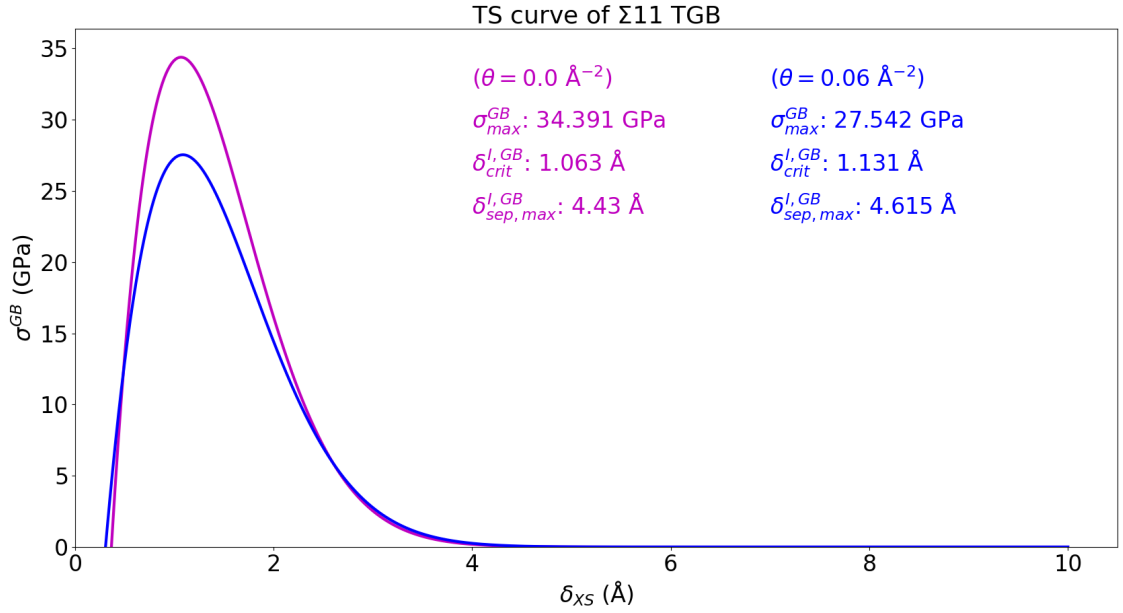


Fig. S11. TS curves for (a) pristine and (b) $\theta = 0.06$ Å^{-2} Σ11 TGB.

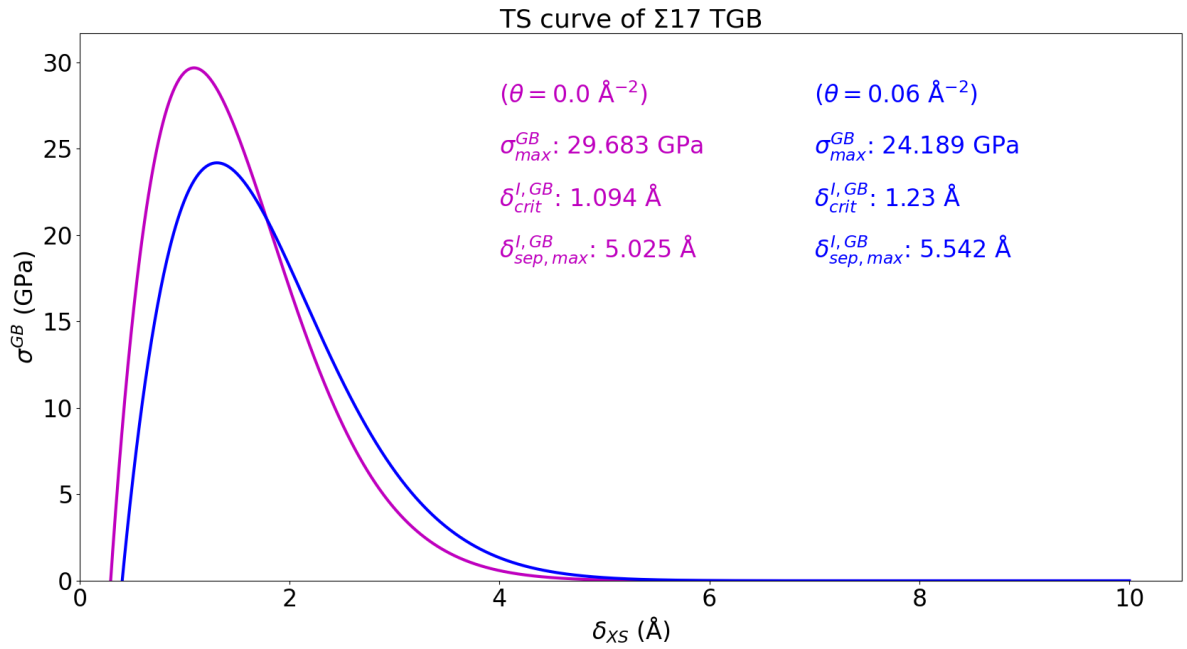


Fig. S12. TS curves for (a) pristine and (b) $\theta = 0.06$ Å^{-2} Σ17 TGB.

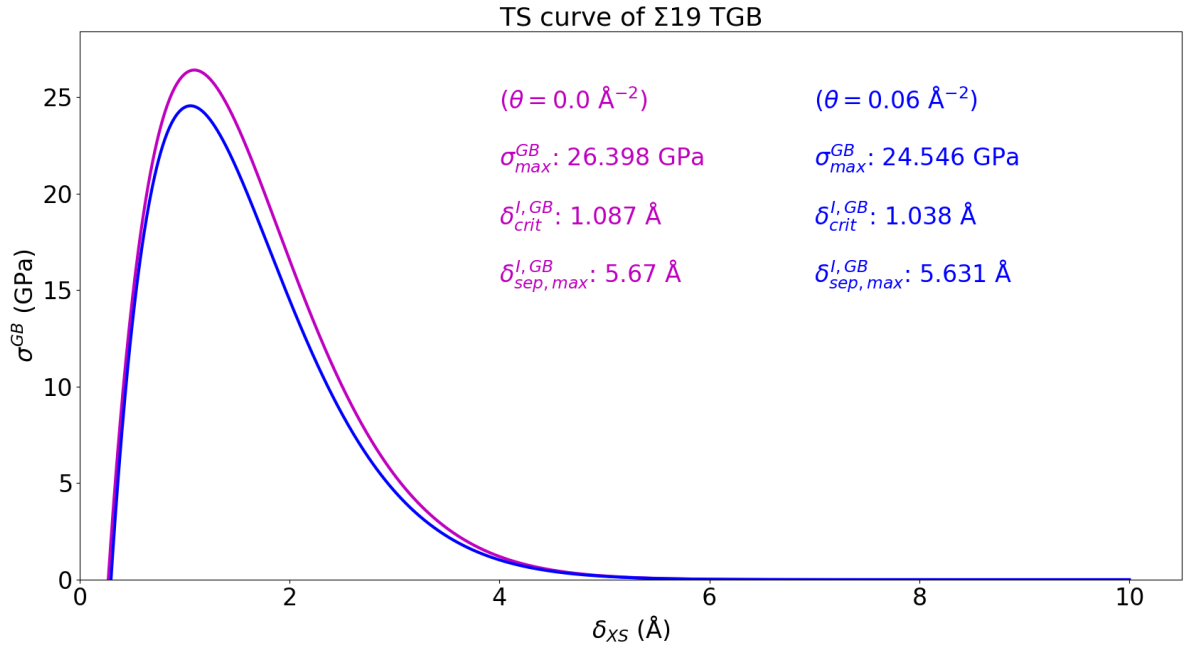


Fig. S13. TS curves for (a) pristine and (b) $\theta = 0.06$ Å^{-2} Σ19 TGB.

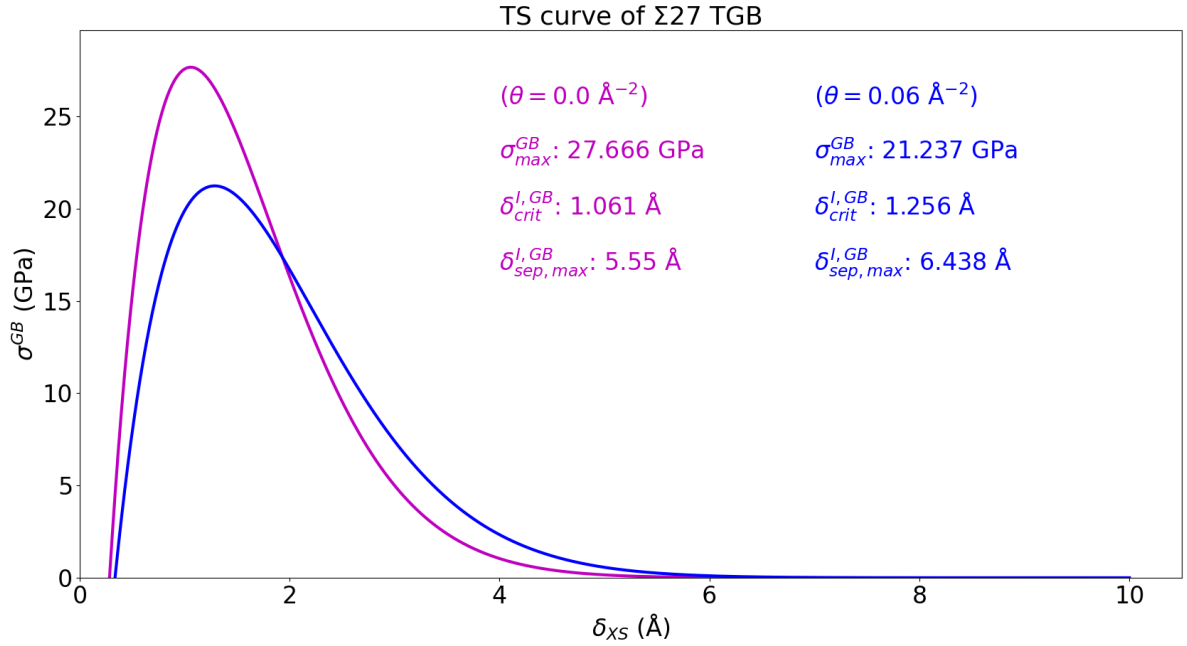


Fig. S14. TS curves for (a) pristine and (b) $\theta = 0.06$ Å^{-2} Σ27 TGB.

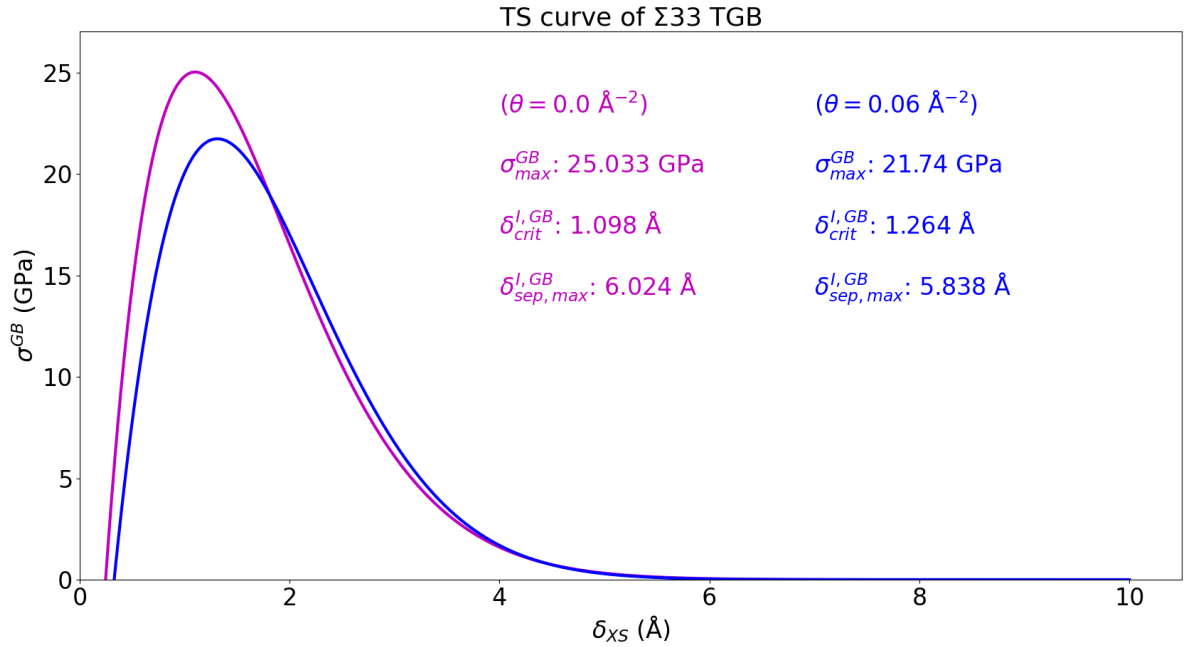


Fig. S15. TS curves for (a) pristine and (b) $\theta = 0.06$ Å^{-2} Σ33 TGB.

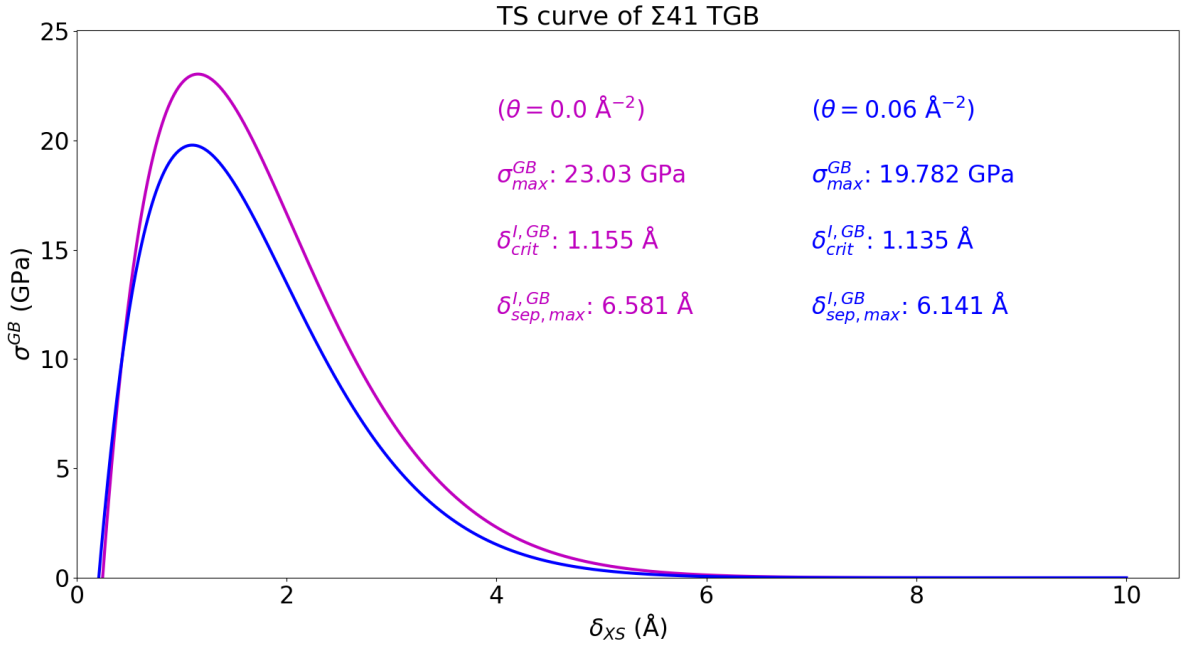


Fig. S16. TS curves for (a) pristine and (b) $\theta = 0.06$ Å^{-2} Σ41 TGB.

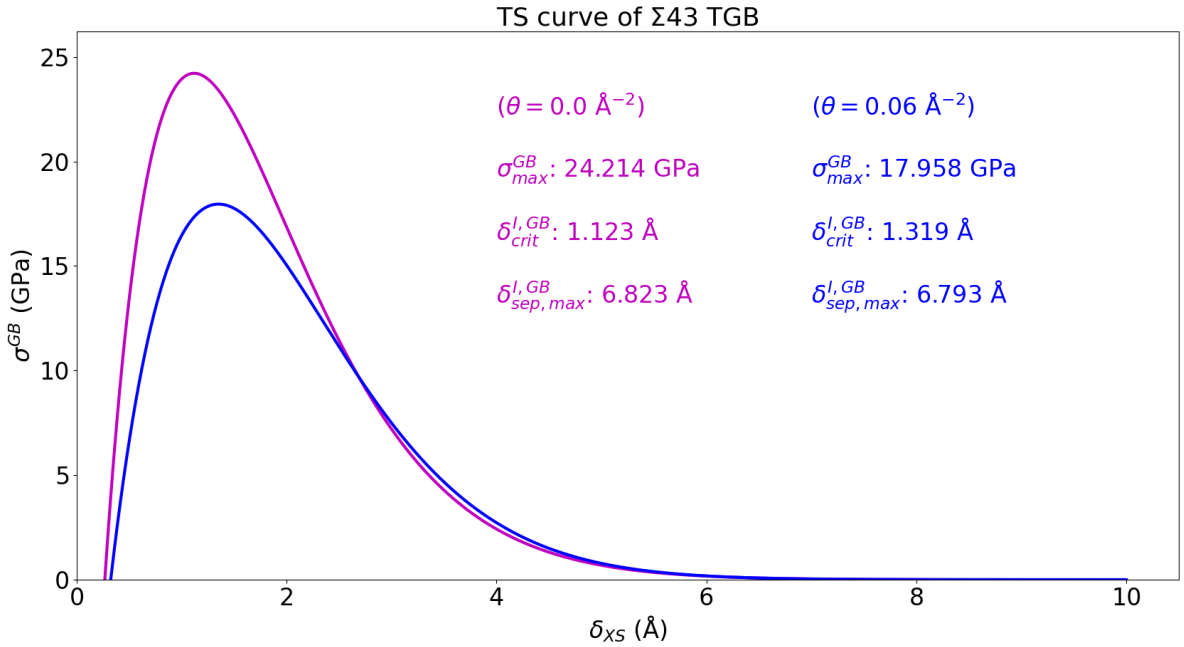


Fig. S17. TS curves for (a) pristine and (b) $\theta = 0.06$ Å^{-2} Σ43 TGB.

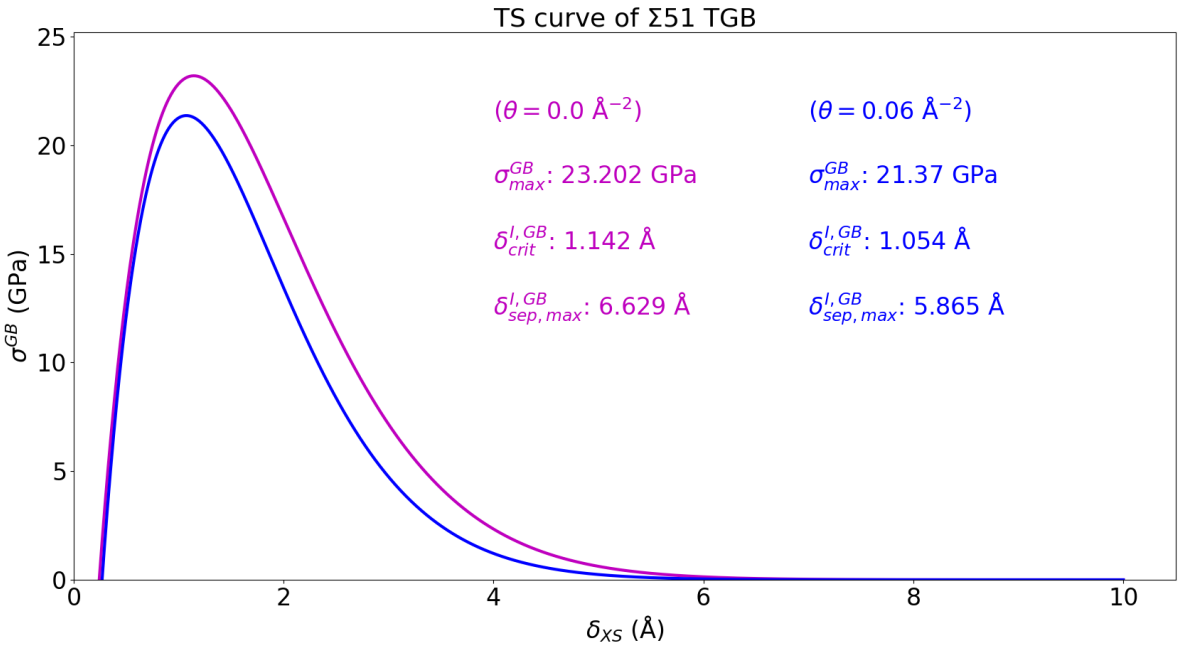


Fig. S18. TS curves for (a) pristine and (b) $\theta = 0.06$ Å^{-2} Σ51 TGB.

Table S2. Maximum/peak stress (σ_{max}^{GB} in units of GPa) in TS curves for the $\langle 110 \rangle$ TGBs considered in the present work. Here, θ stands for P impurities coverage.

GB	σ_{coh}^{GB}	
Σ	$\theta = 0.0$ Å^{-2}	$\theta = 0.06$ Å^{-2}
Σ51	23.202	21.370
Σ33	25.033	21.740
Σ19	26.398	24.546
Σ27	27.666	21.237
Σ9	38.287	26.598
Σ11	34.391	27.542
Σ41	23.030	19.782
Σ3	36.342	29.653
Σ43	24.214	17.958
Σ17	29.683	24.189