Electronic Supplementary Information

A new computational strategy to calculate the edge energy of a relaxed step. Calcite ($CaCO_3$) as a case study

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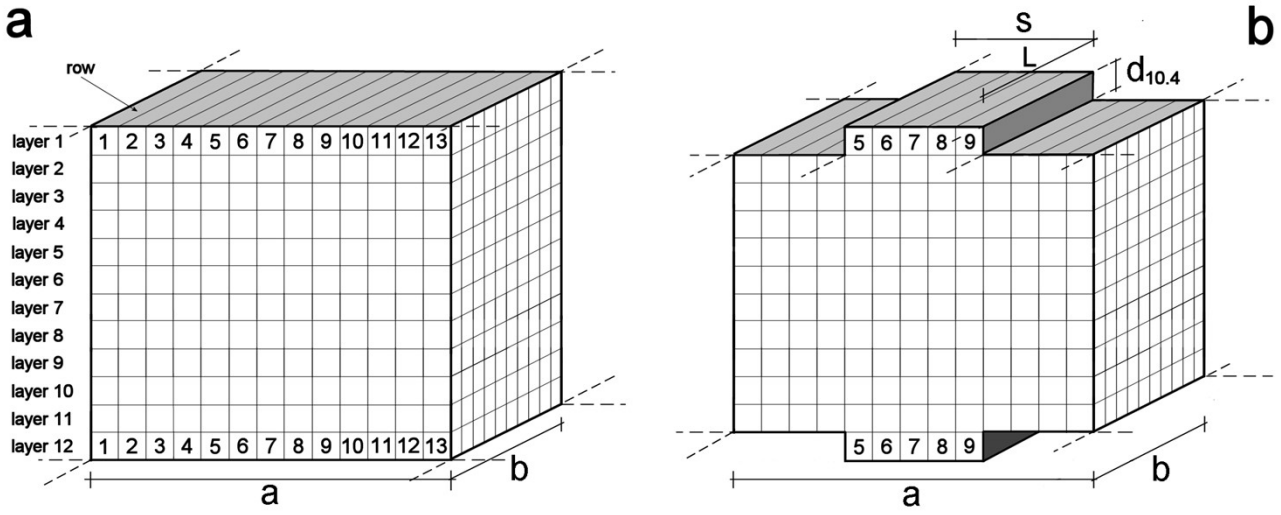

Figure S1. Kossel's crystal is used to exemplify the construction of two steps of height $d_{10.4}$ on the top and bottom crystal surface of a slab of calcite for performing quantum-mechanical geometry optimizations. (a) Twelve-layers (10.4) slab is cut from the optimized bulk structure of calcite. (b) Steps delimited by two [uvw] edges parallel to cell parameter *b* are generated by deleting rows 1-4 and 10-13 in the layers 1 and 12. *S* and *L* are the width and length of the step, respectively. Top and bottom surfaces of the slab (with step) are be put in relation by either an inversion center or a mirror plane to cancel out the dipole moment and allowing quantum-mechanical calculations.

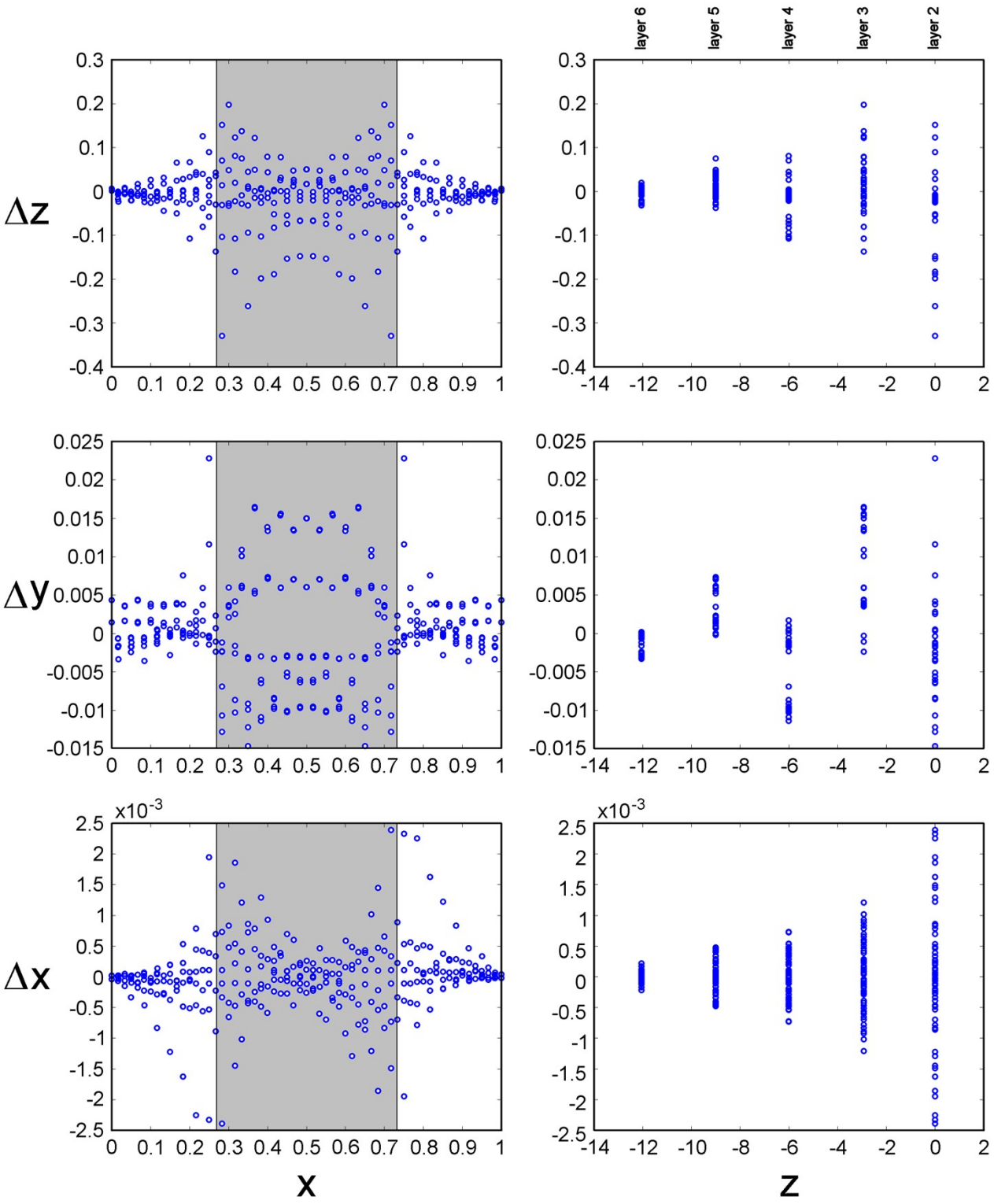

Figure S2. ΔX, ΔY and ΔZ as a function of X (fractional coordinates) and Z (cartesian coordinates, Å) for the $[4\bar{2}1]_{Ca}$ step on (10.4) surface. In the left column, the grey area indicates the location of the step along X. In the right column, Z = 0 is the $d_{10.4}$ layer just below the step (i.e., layer 2) and Z ~ -12 Å is the last layer in region 1 (i.e., layer 6).

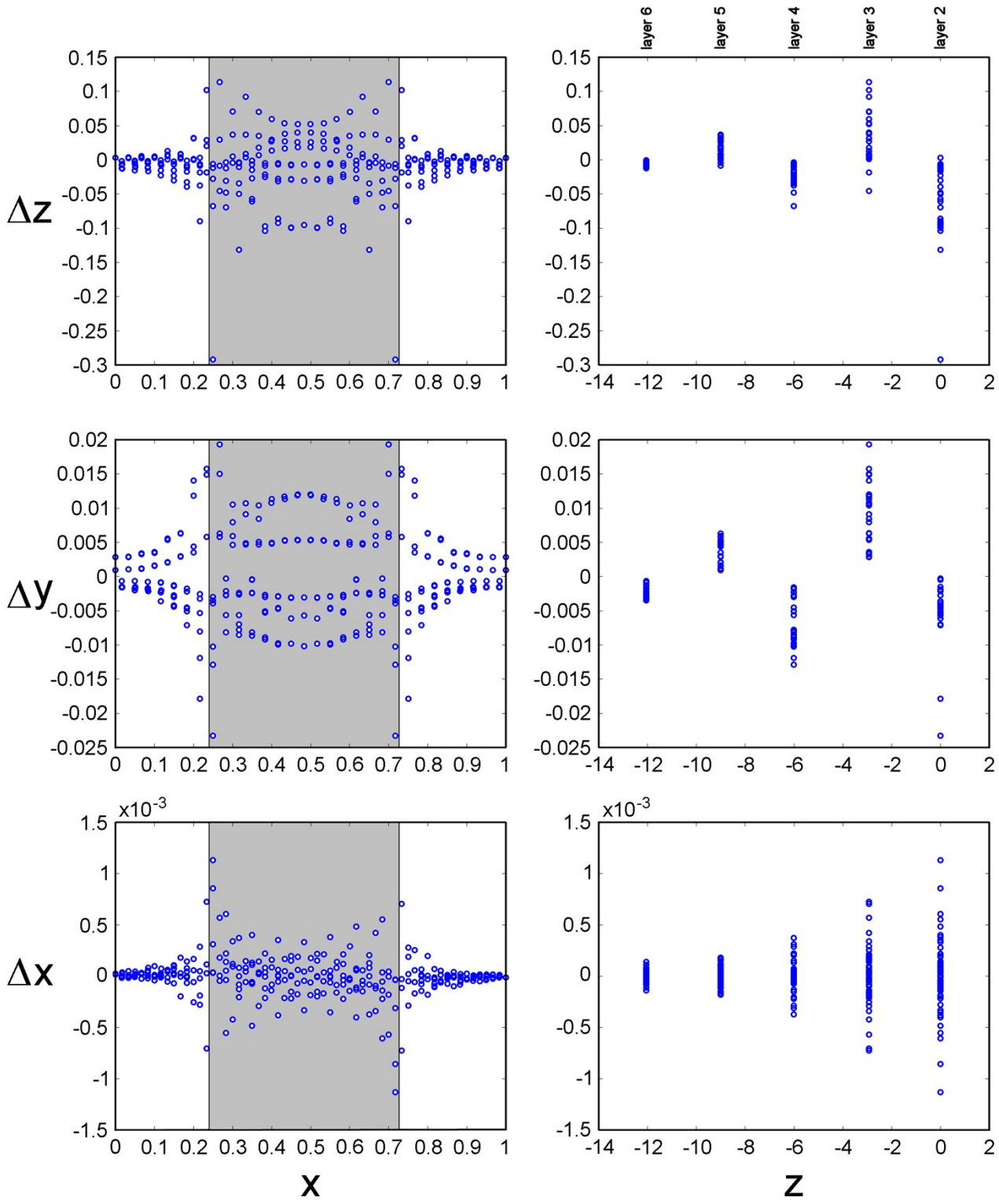

Figure S3. ΔX, ΔY and ΔZ as a function of X (fractional coordinates) and Z (cartesian coordinates, Å) for the $[4\bar{2}1]_{CO3(A)}$ step on (10.4) surface. In the left column, the grey area indicates the location of the step along X. In the right column, Z = 0 is the $d_{10.4}$ layer just below the step (i.e., layer 2) and Z ~ -12 Å is the last layer in region 1 (i.e., layer 6).

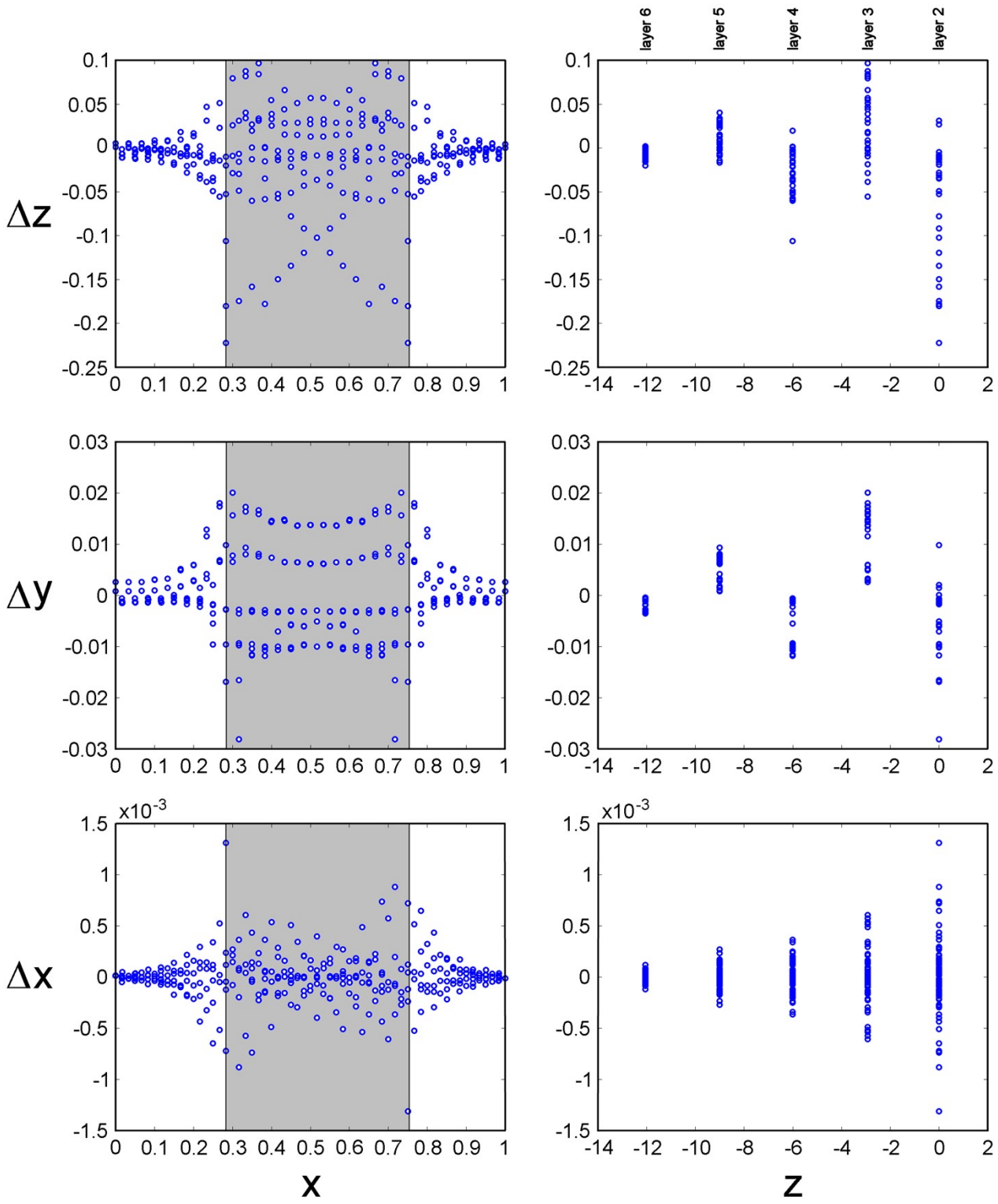

Figure S4. ΔX, ΔY and ΔZ as a function of X (fractional coordinates) and Z (cartesian coordinates, Å) for the $[4\bar{2}1]_{CO3(B)}$ step on (10.4) surface. In the left column, the grey area indicates the location of the step along X. In the right column, Z = 0 is the $d_{10.4}$ layer just below the step (i.e., layer 2) and Z ~ -12 Å is the last layer in region 1 (i.e., layer 6).

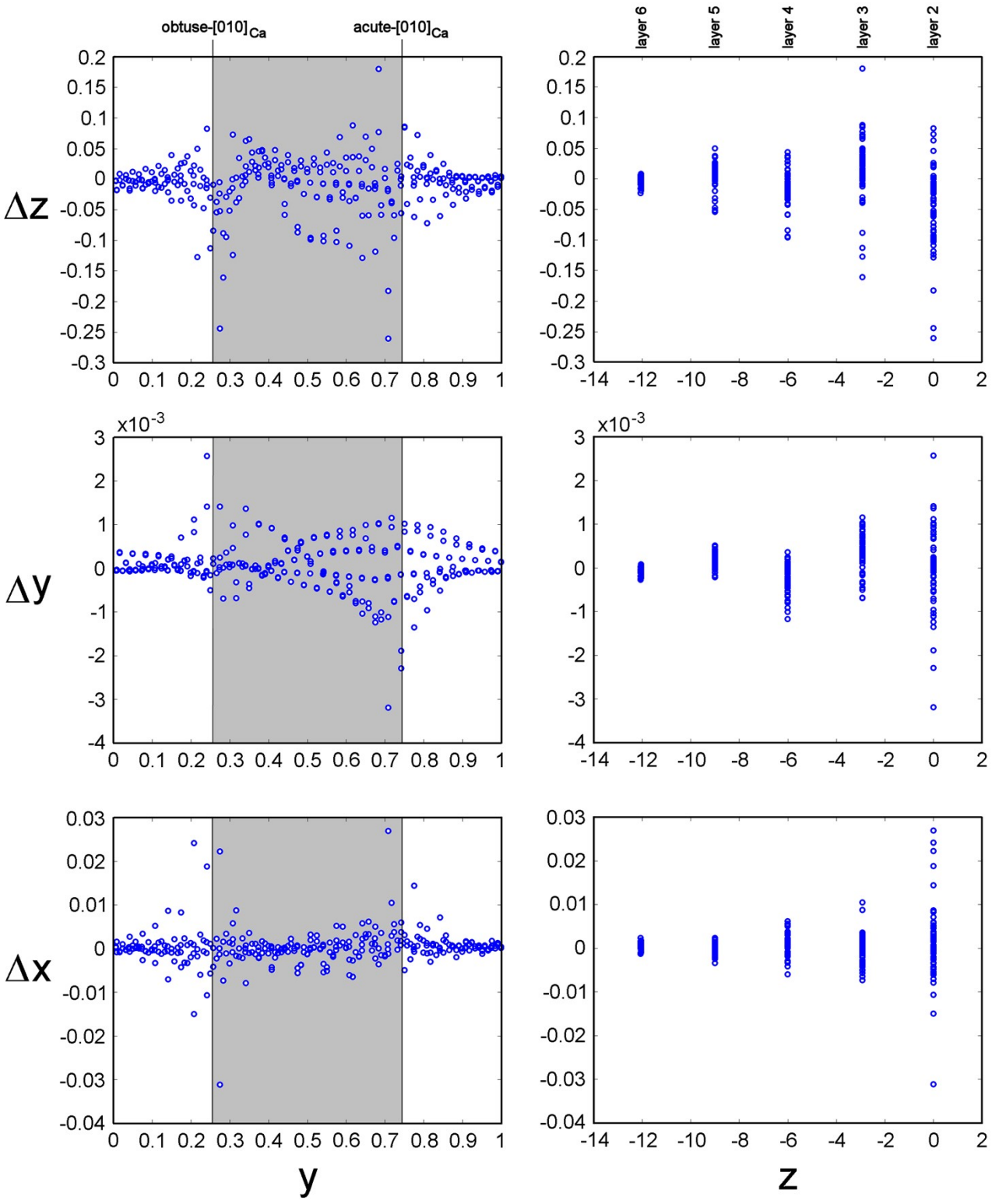

Figure S5. ΔX, ΔY and ΔZ as a function of X (fractional coordinates) and Z (cartesian coordinates, Å) for the $[010]_{Ca}$ step on (10.4) surface. In the left column, the grey area indicates the location of the step along Y. In the right column, Z = 0 is the $d_{10.4}$ layer just below the step (i.e., layer 2) and Z ~ -12 Å is the last layer in region 1 (i.e., layer 6).

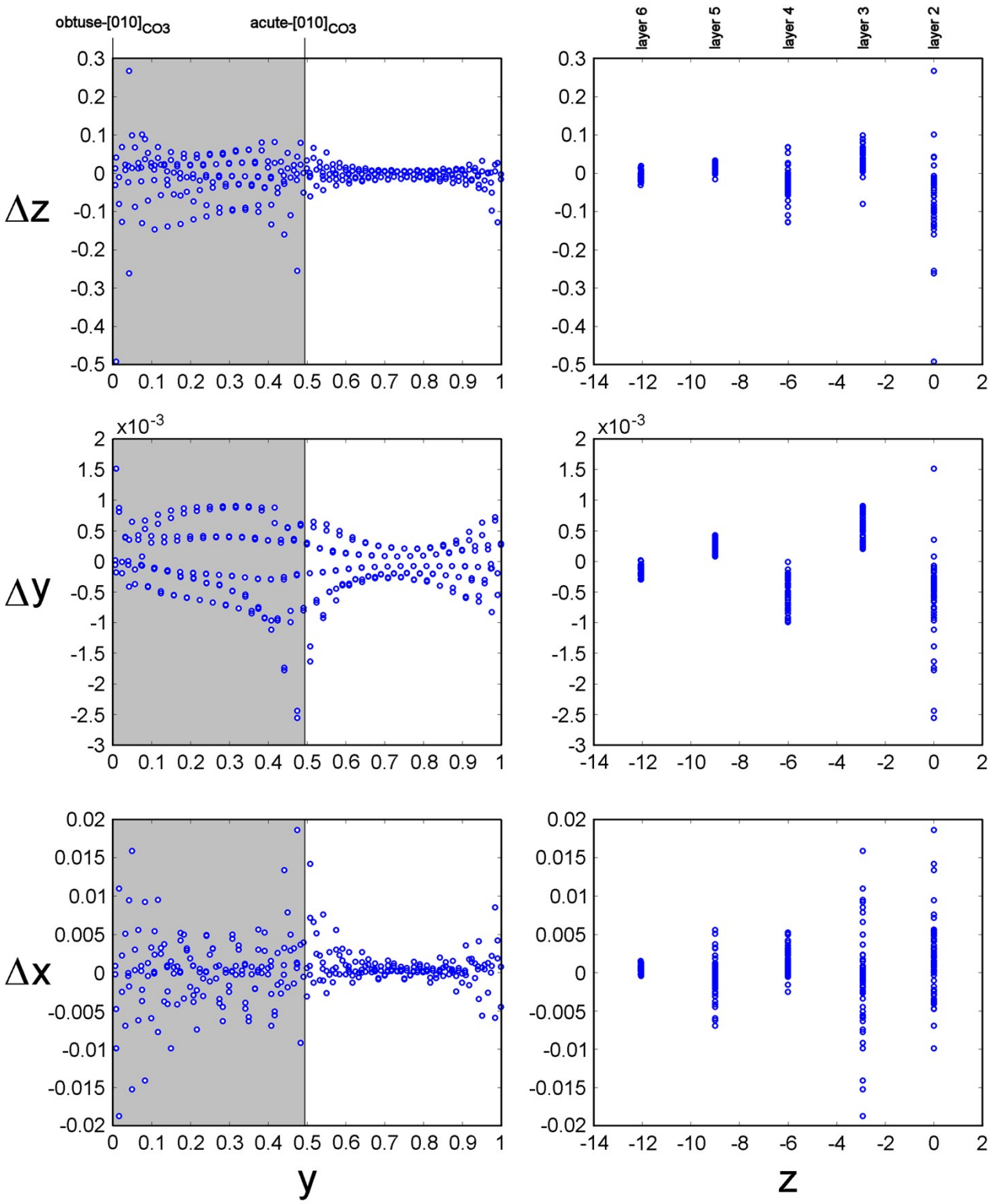

Figure S6. ΔX, ΔY and ΔZ as a function of X (fractional coordinates) and Z (cartesian coordinates, Å) for the $[010]_{CO3}$ step on (10.4) surface. In the left column, the grey area indicates the location of the step along Y. In the right column, Z = 0 is the $d_{10.4}$ layer just below the step (i.e., layer 2) and Z ~ -12 Å is the last layer in region 1 (i.e., layer 6).