

FIGURE 1. Single pleated sheet illustrating the concepts of Z-chains, ridges, and valleys. Z-chains donating 'E' have their oxygens colored red (except O*). Z-chains donating 'W' have their oxygens colored blue.

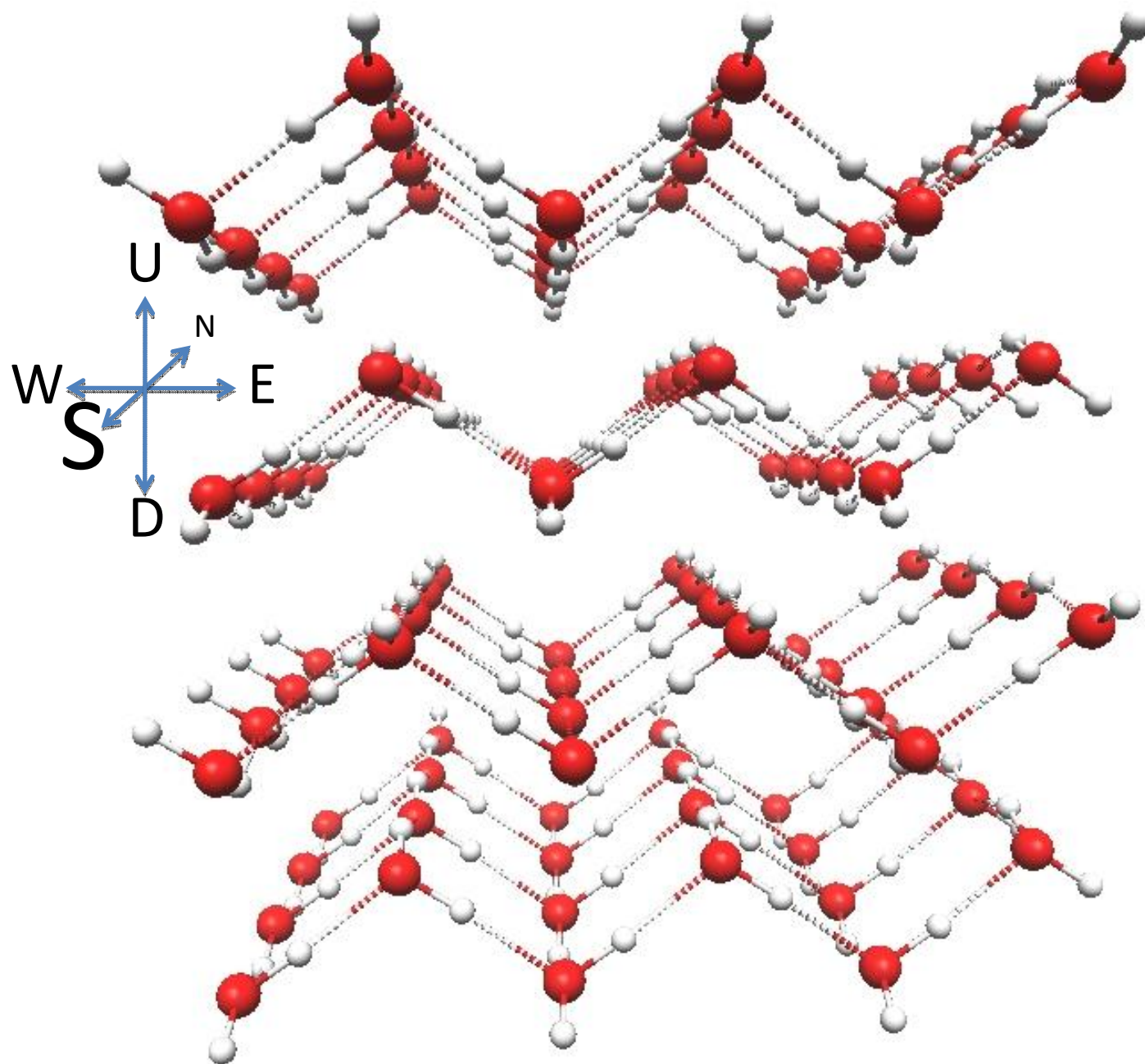
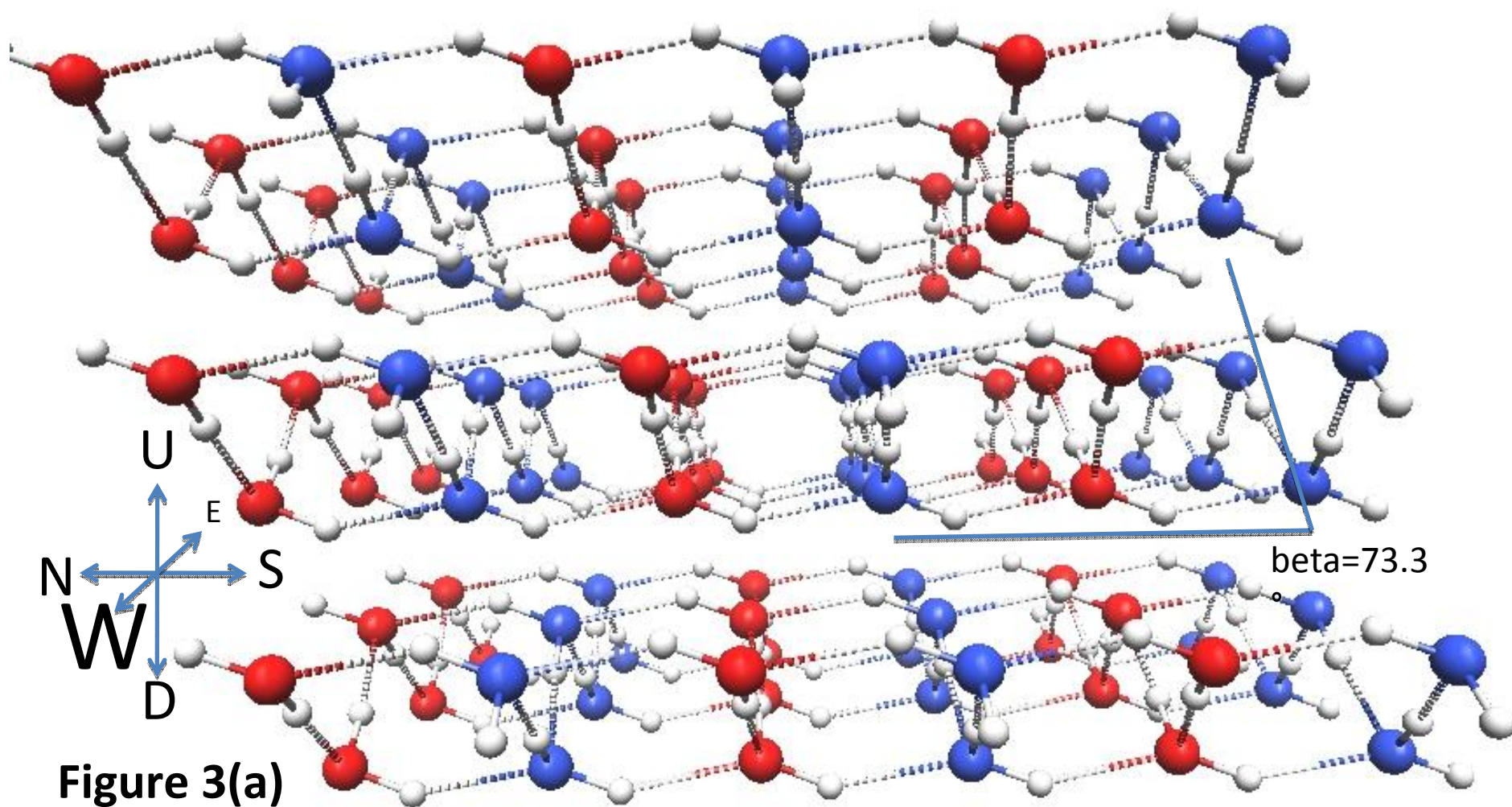


FIGURE 2. NE/S/E/SW, an example of a PSW Category 2 lattice. This view highlights nesting of the ridges and valleys.



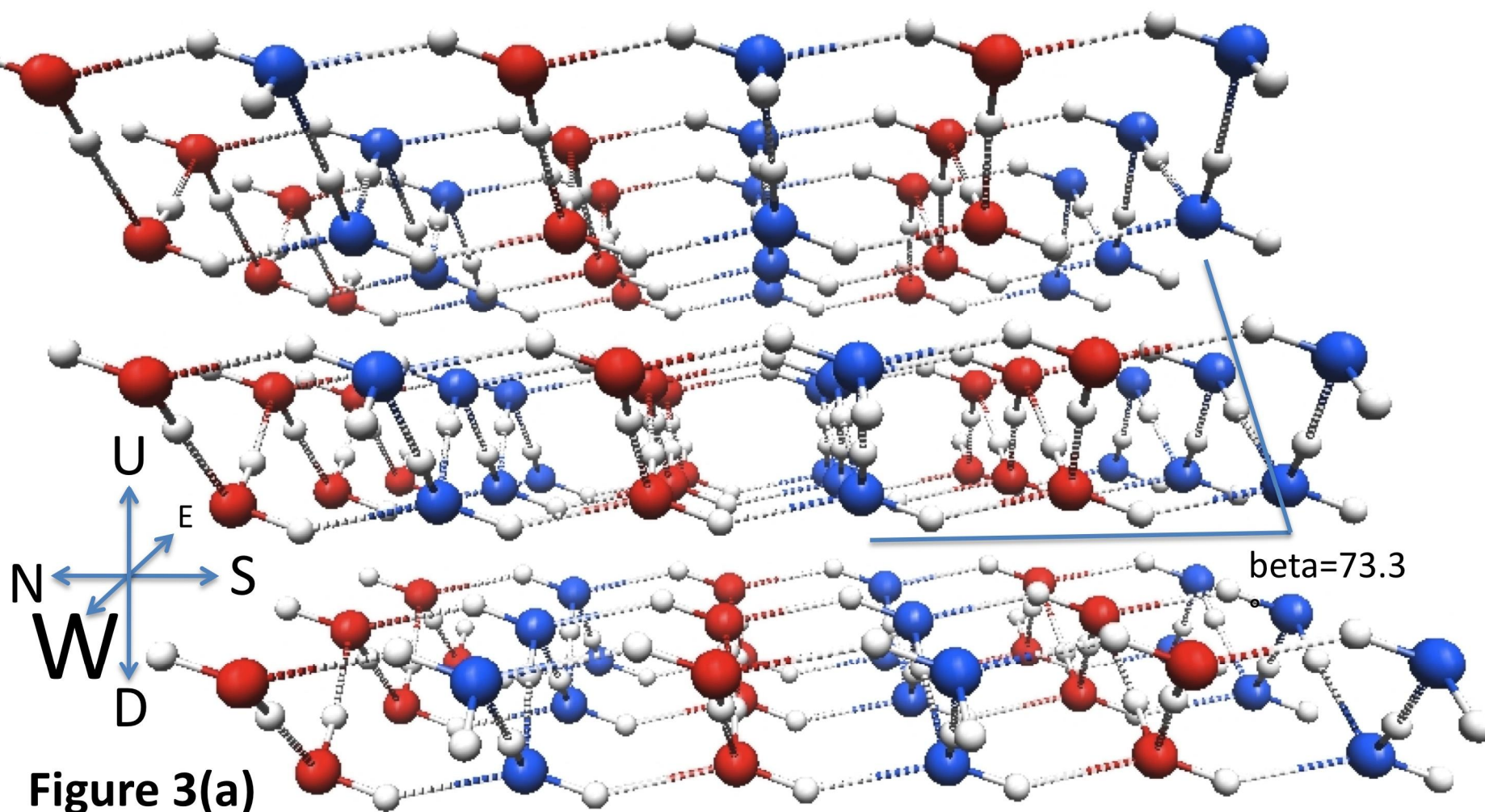


FIGURE 3. Illustration of PSW Category 1 monoclinic lattices. (a) and (b) are local minima on the same SPES, using the same monoclinic lattice but with different “beta” angles. Figure 3(a) is the proposed microlattice structure for VHDA. For clarity E-going Z-chains’ O’s are red and W-going Z-chains’ O’s are blue. (a) NE/S/W/NE. (b) NE/S/W/NW.

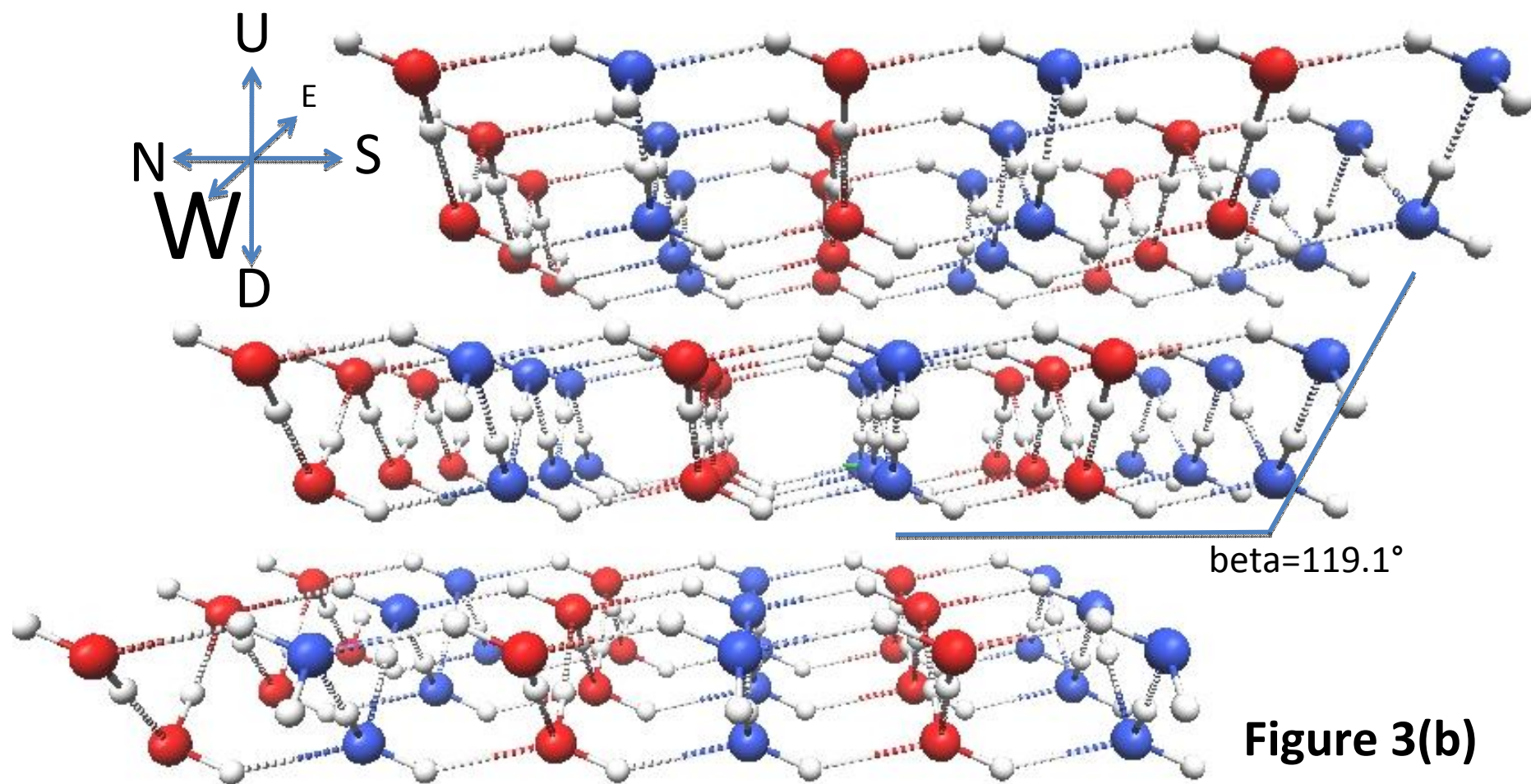


Figure 3(b)

Figure 4(a)

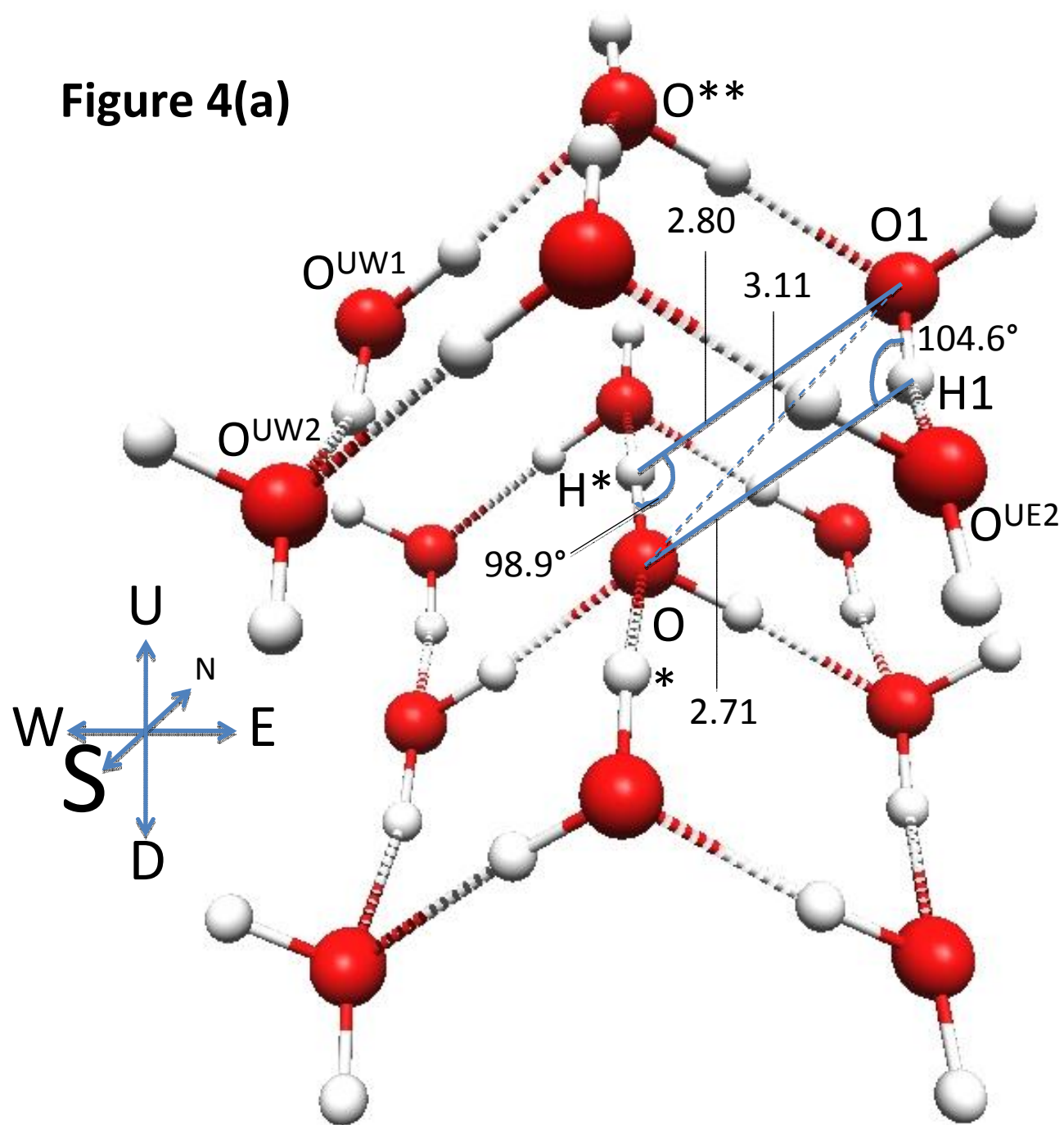
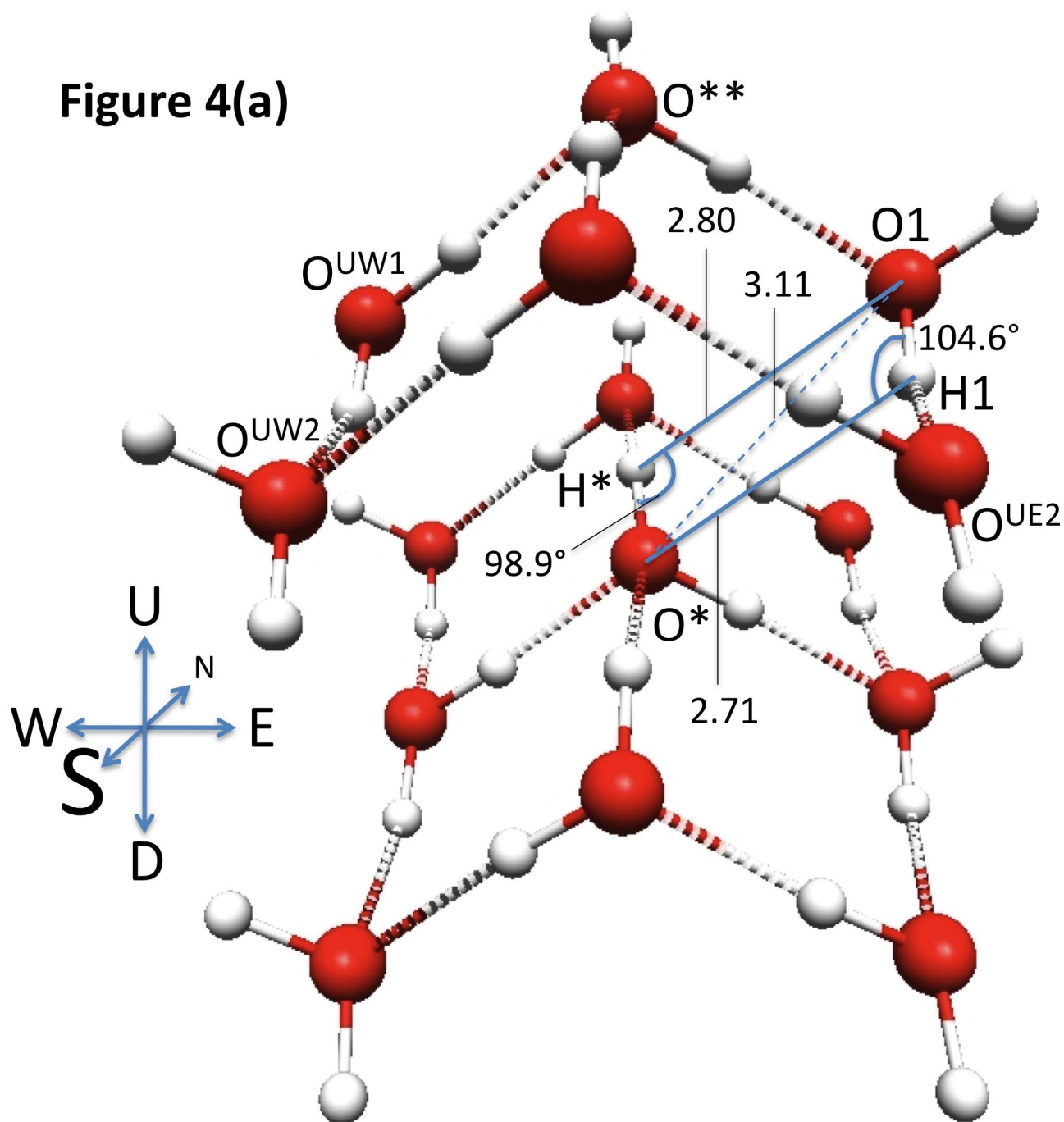
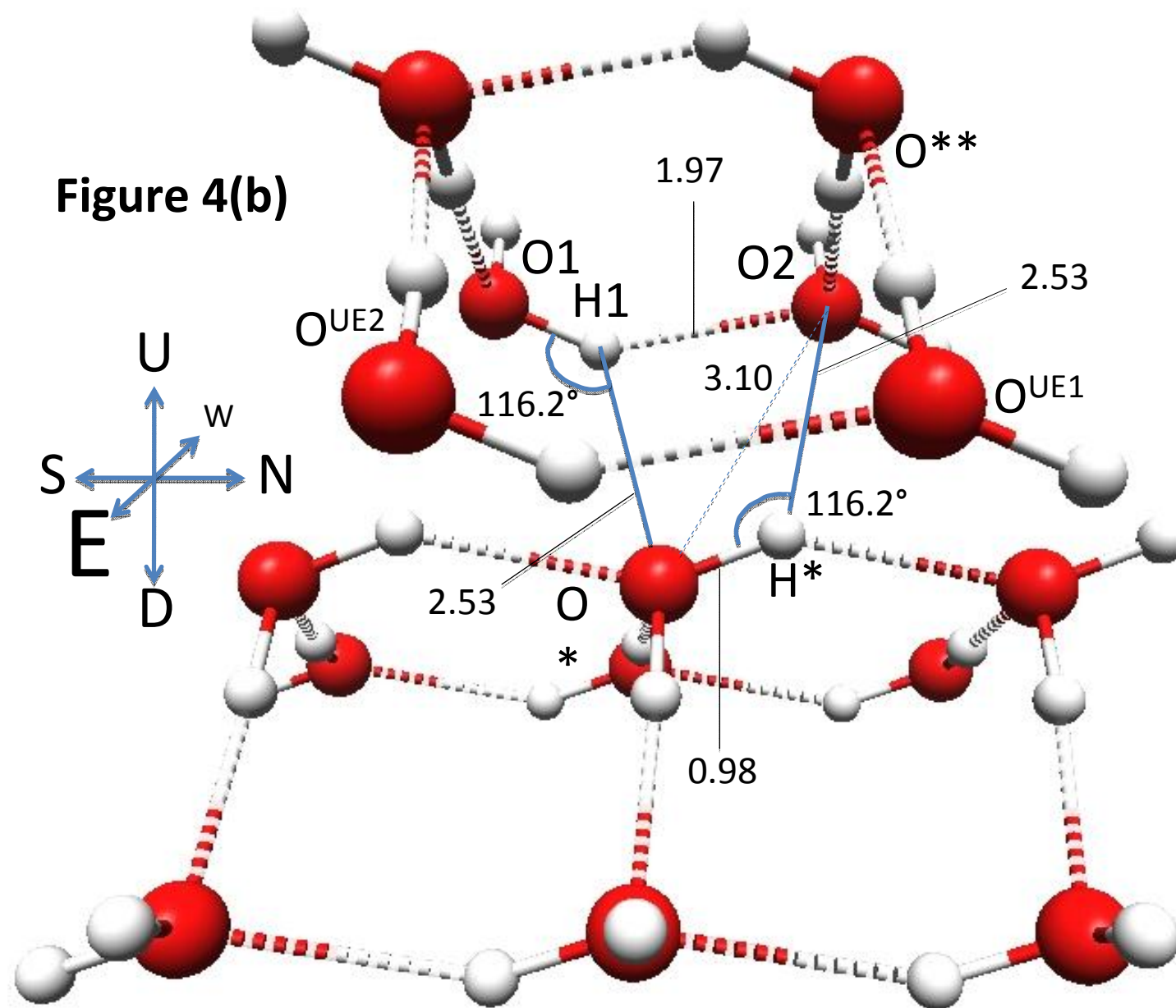


FIGURE 4. Illustration of geometries for the proposed concept of dispersion bond. (a) Category 1 bond setup. Blow-up of a neighborhood of an index O^* of NE/S/W/NE (Fig. 3(a)) viewed from S toward N, illustrating the $O^*-H^*-O1-H1$ parallelogram with some angles and distances. Here O1 is the next-sheet neighbor O^{UE1} . (b) Category 2 bond setup. Blow-up of a neighborhood of an index O^* of NE/S/E/SW (Fig. 2) viewed from E, illustrating the $H1-O^*-H^*-O2$ trapezoid. Here O1 and O2 are the next-sheet neighbors O^{UW2} and O^{UW1} respectively.





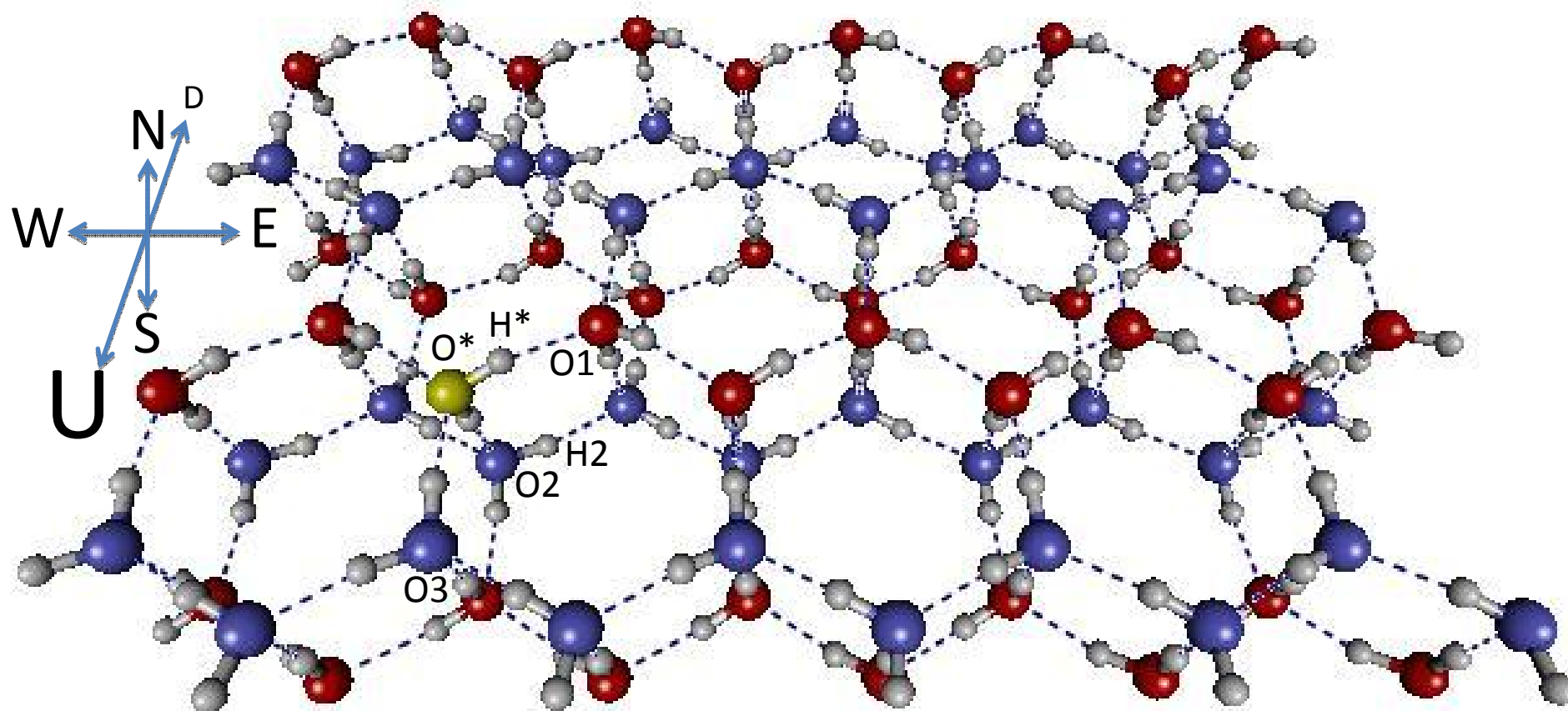


FIGURE 5. Illustration of a single hexagonal bilayer. Each Z-chain has either all red (except O*) or all blue O's. For this lattice, the red O's are all joining (J) and the blue O's are all facial (F). Lattice notation: let the index O* (yellow color) be on an E-going Z-chain, on the N face of the bilayer, and joining (J). This lattice is "EJ/JEW" because same-Z-chain neighbor O1 is J and the adjacent chains' directions given by donors at O2 and O3 are E and W respectively.

Figure 6(a)

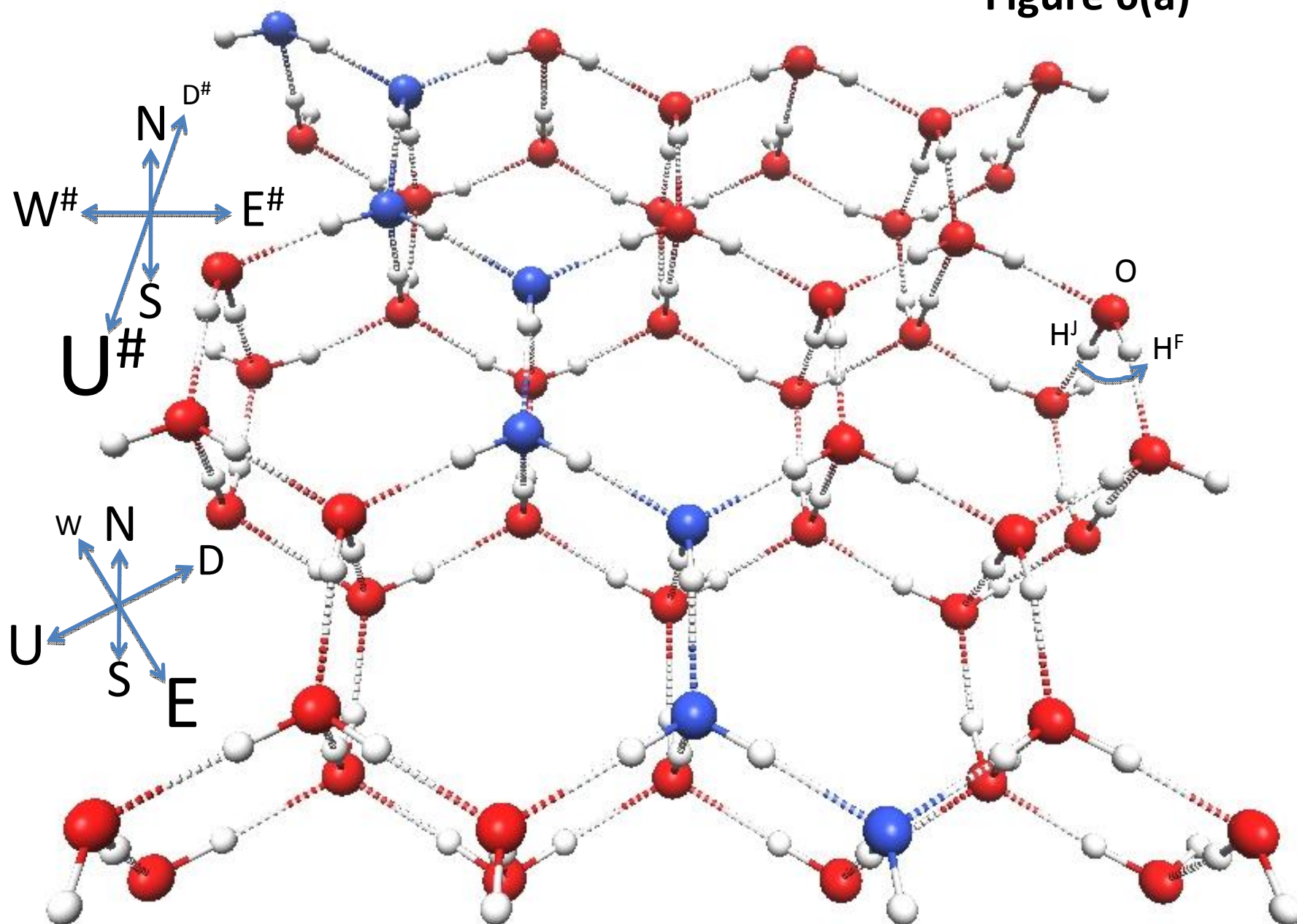


Figure 6(a)

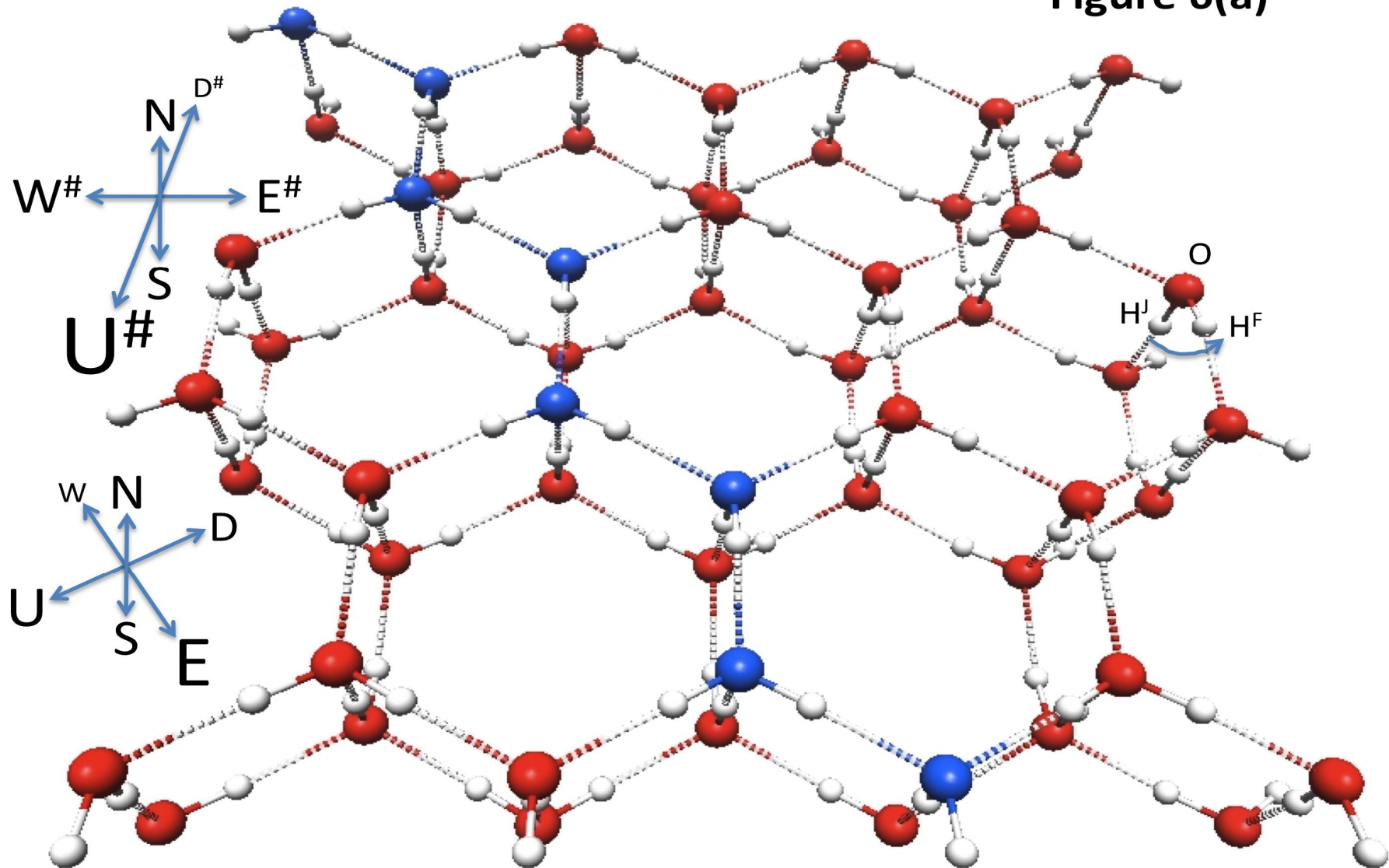


FIGURE 6. Illustration of HBW lattice EJ/FWE. (a) Single bilayer. Note planes of reflection symmetry. One E-going Z-chain is colored blue and both coordinate frames are depicted. (b) EJ/FWEa, the proposed microlattice structure for uHDA. (c) EJ/FWEb, the proposed microlattice structure for eHDA.

Figure 6(b)

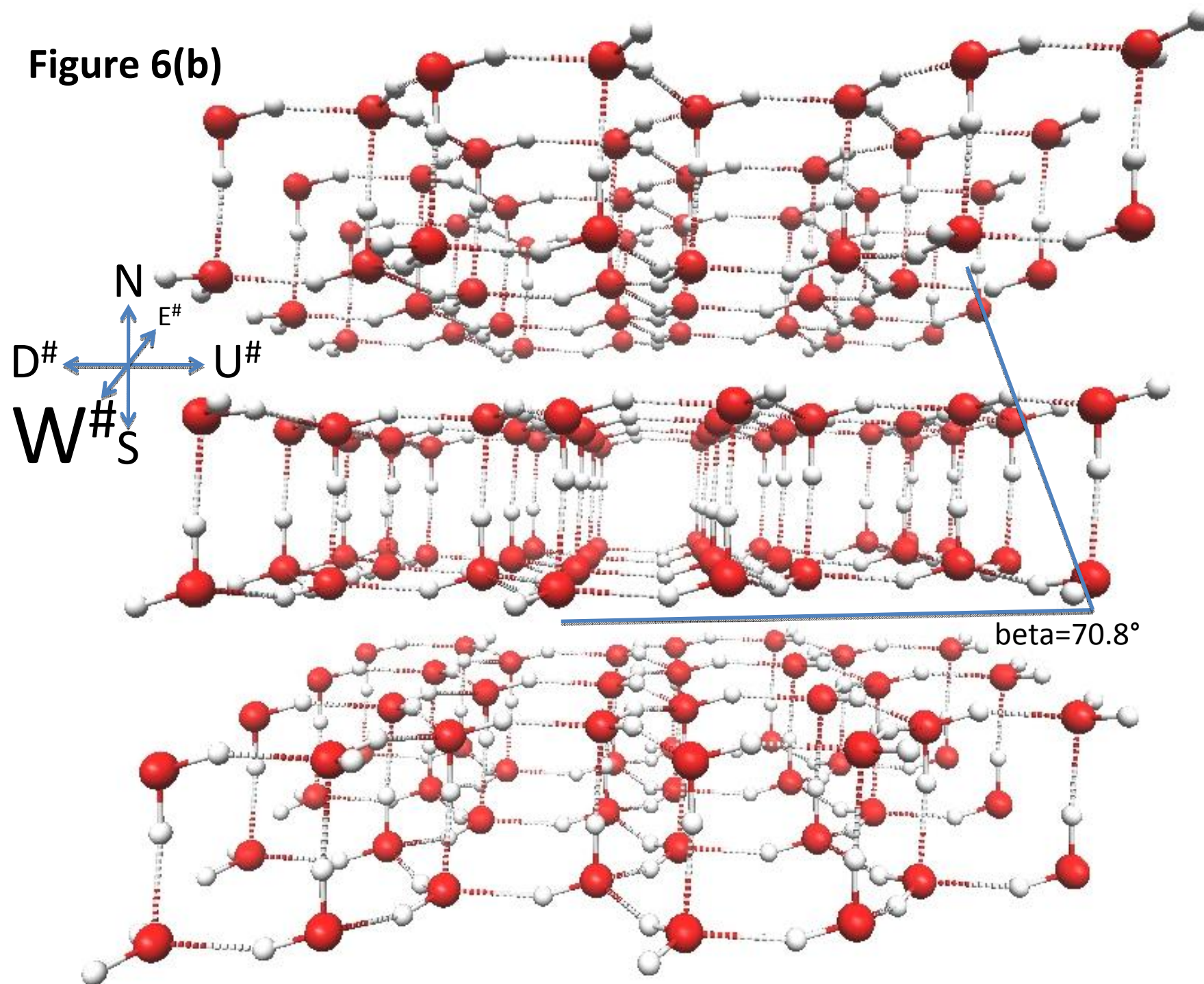


Figure 6(c)

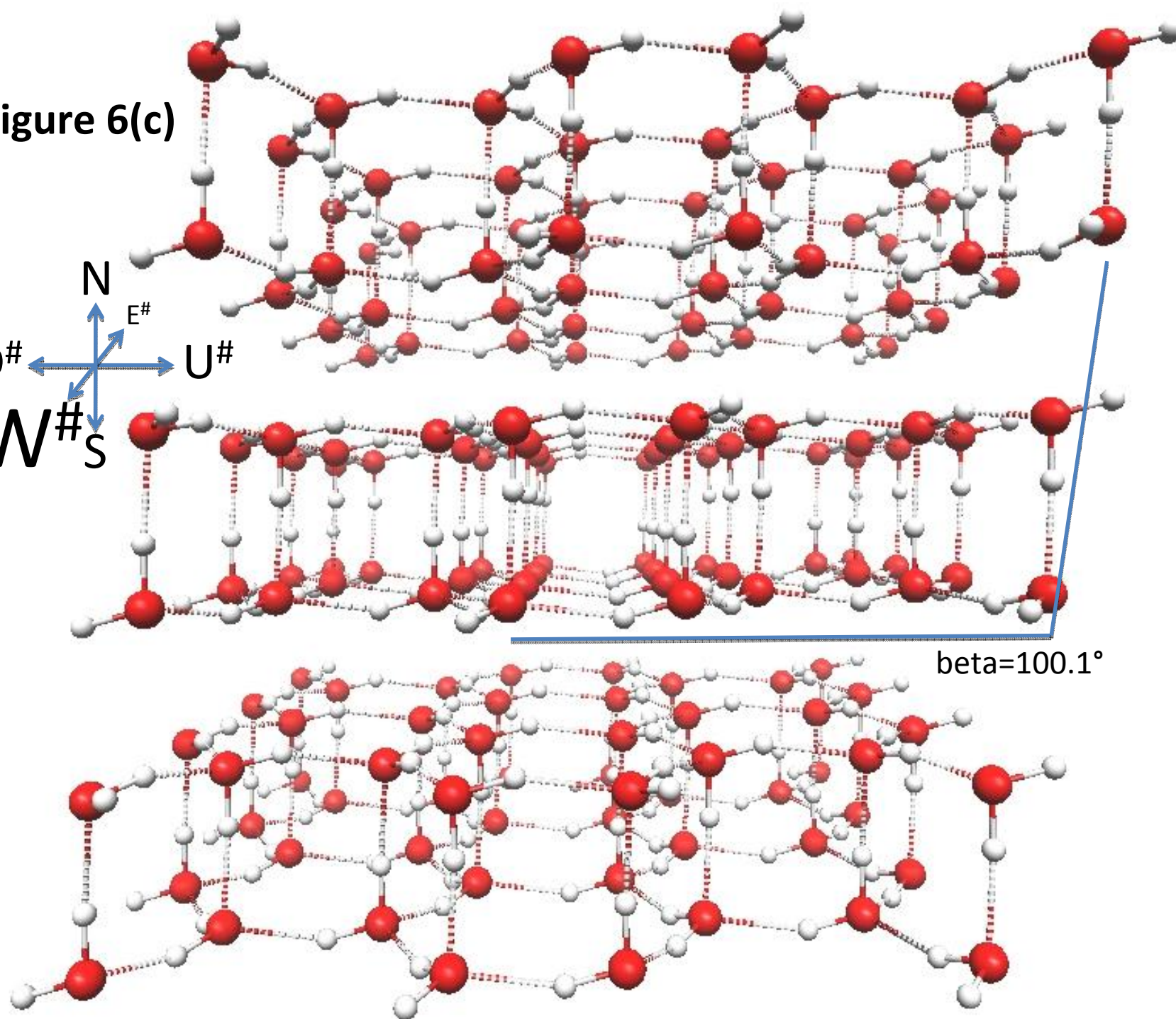
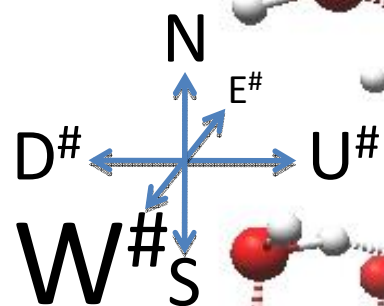
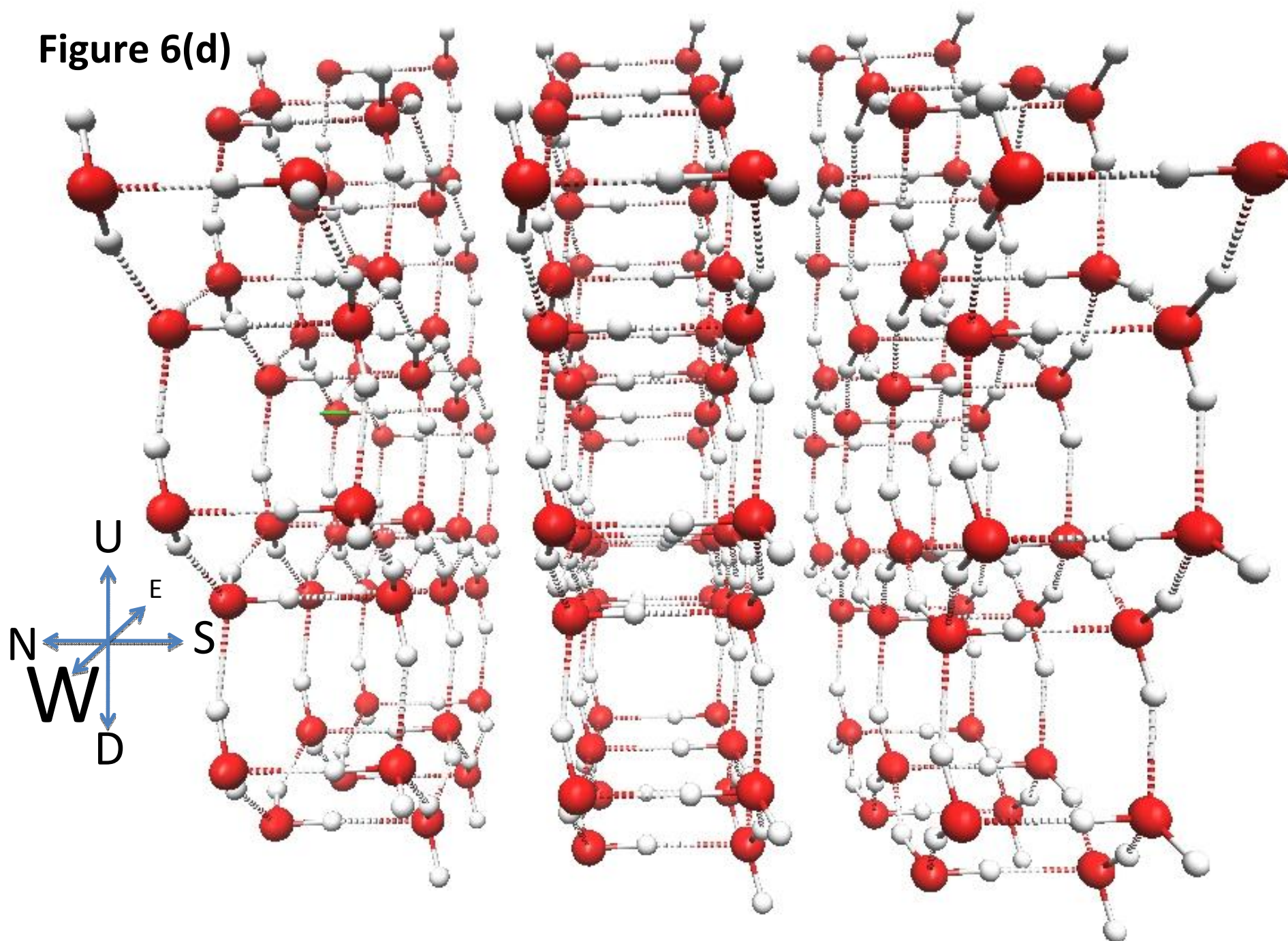


Figure 6(d)



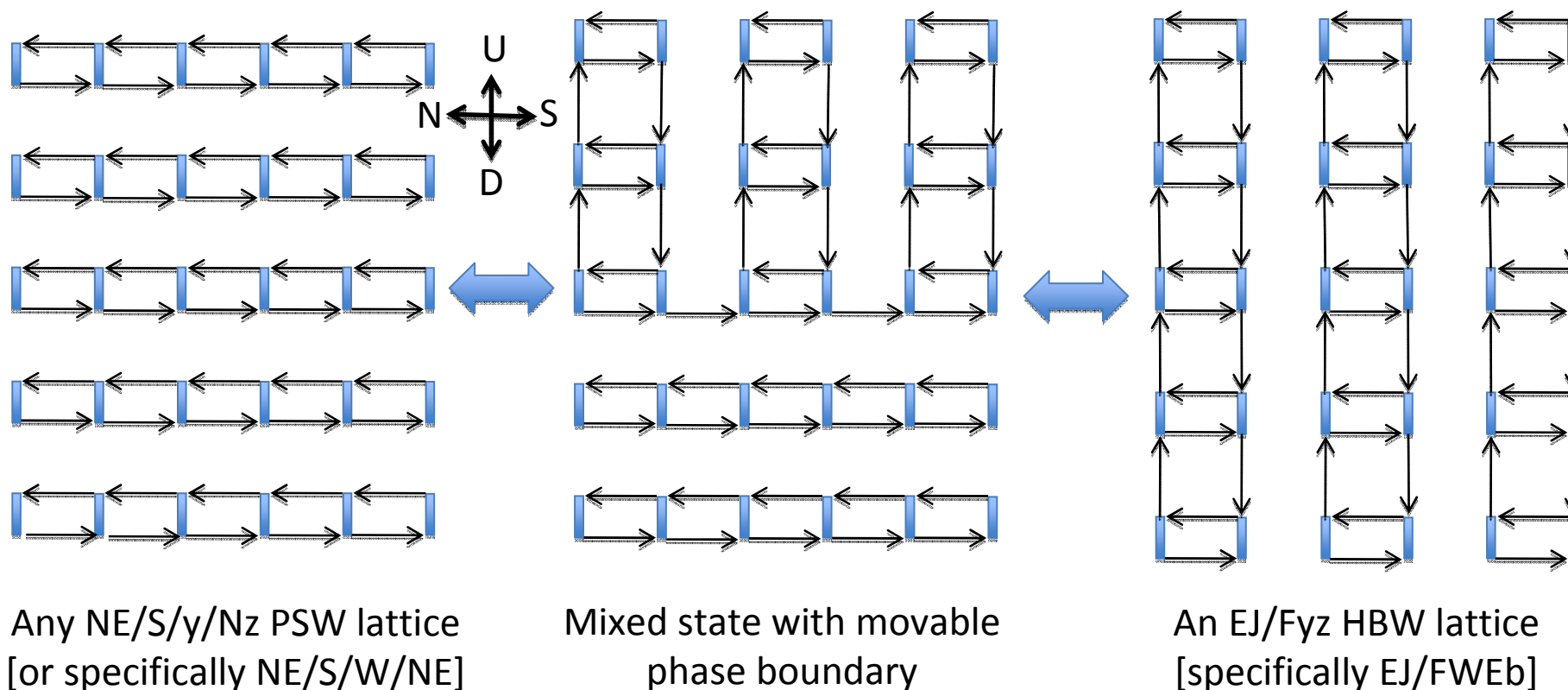


FIGURE 7. Schematic representation of the interconversion of PSW (NE/S/y/Nz) and HBW (EJ/Fyz): Orthographic projection onto the NS-UD plane. Small rectangles represent Z-chains going E or W, with internal H-bonds suppressed for greater clarity. H-bonds external to the Z-chains are represented by arrows.

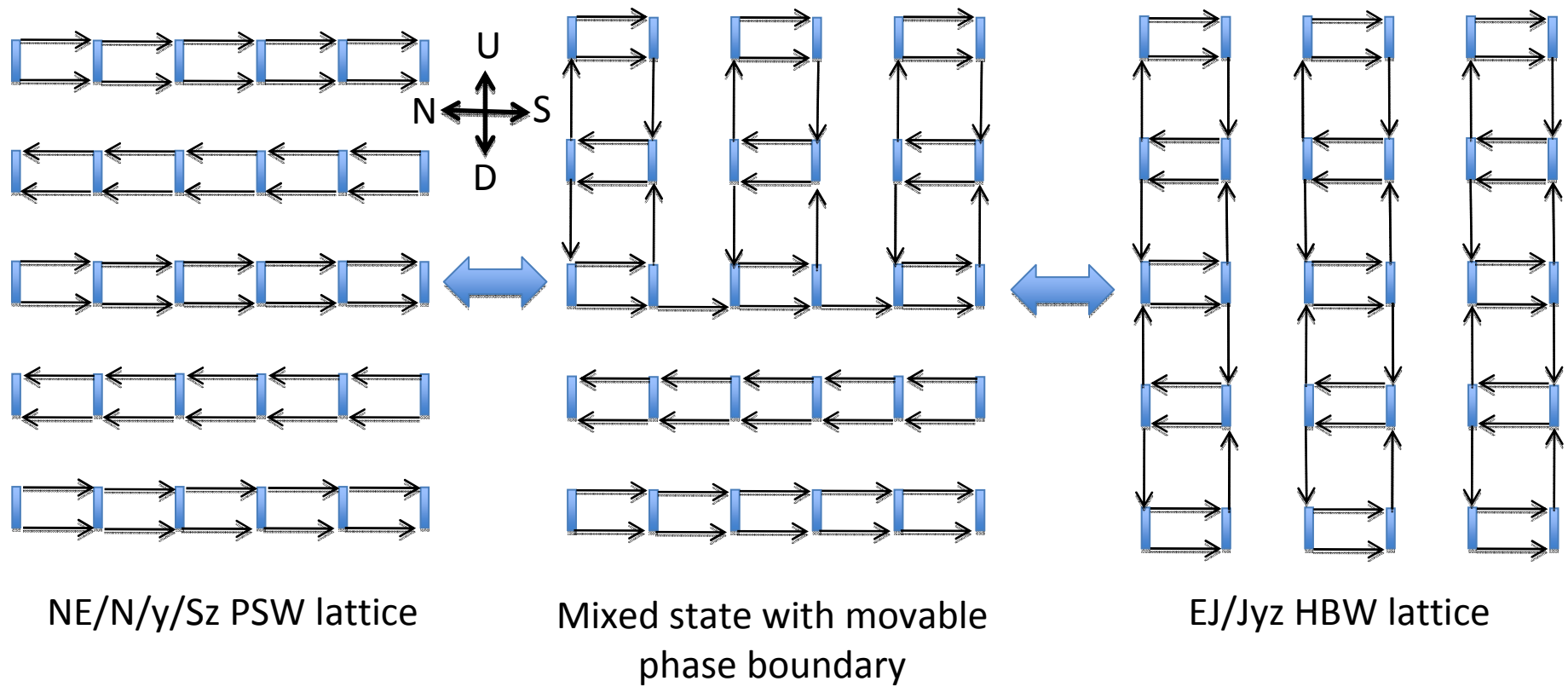


FIGURE 8. Schematic representation of the interconversion of PSW (NE/N/y/Sz) and HBW (EJ/Jyz).

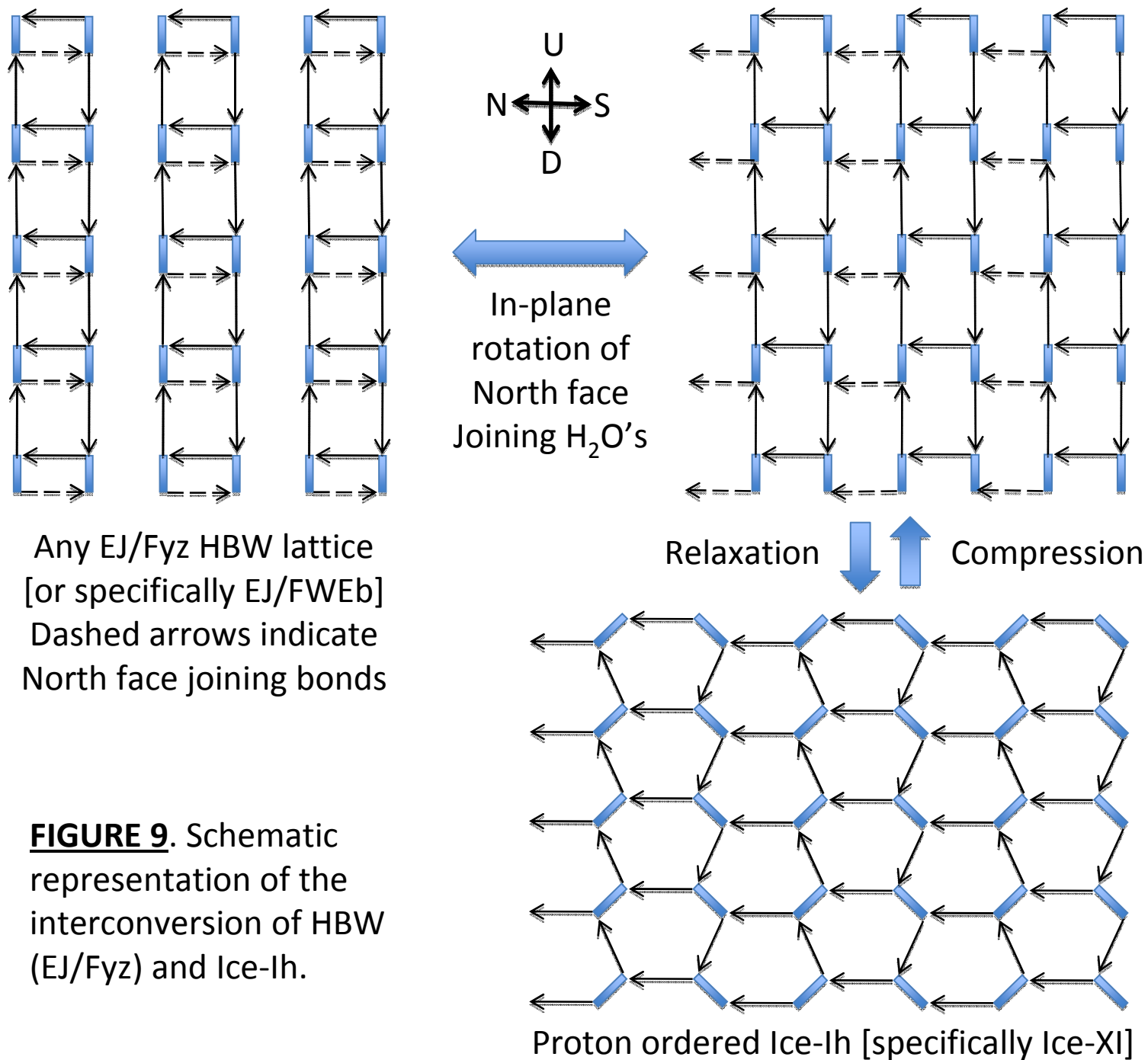
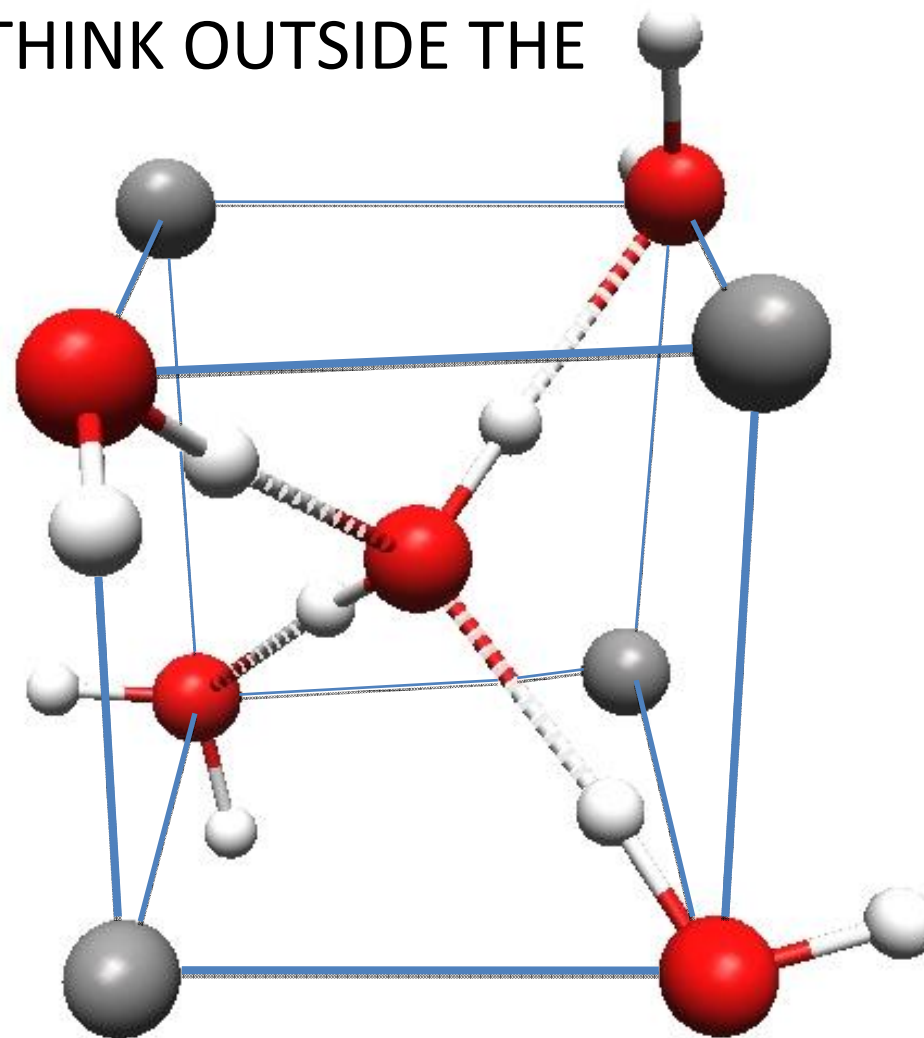


FIGURE 9. Schematic representation of the interconversion of HBW (EJ/Fyz) and Ice-Ih.

THINK OUTSIDE THE



TETRAHEDRAL BOX

