

Supporting Information

Vacancy Diffusion Barriers in TaON and Ta₃N₅ Water-Splitting Photocatalysts

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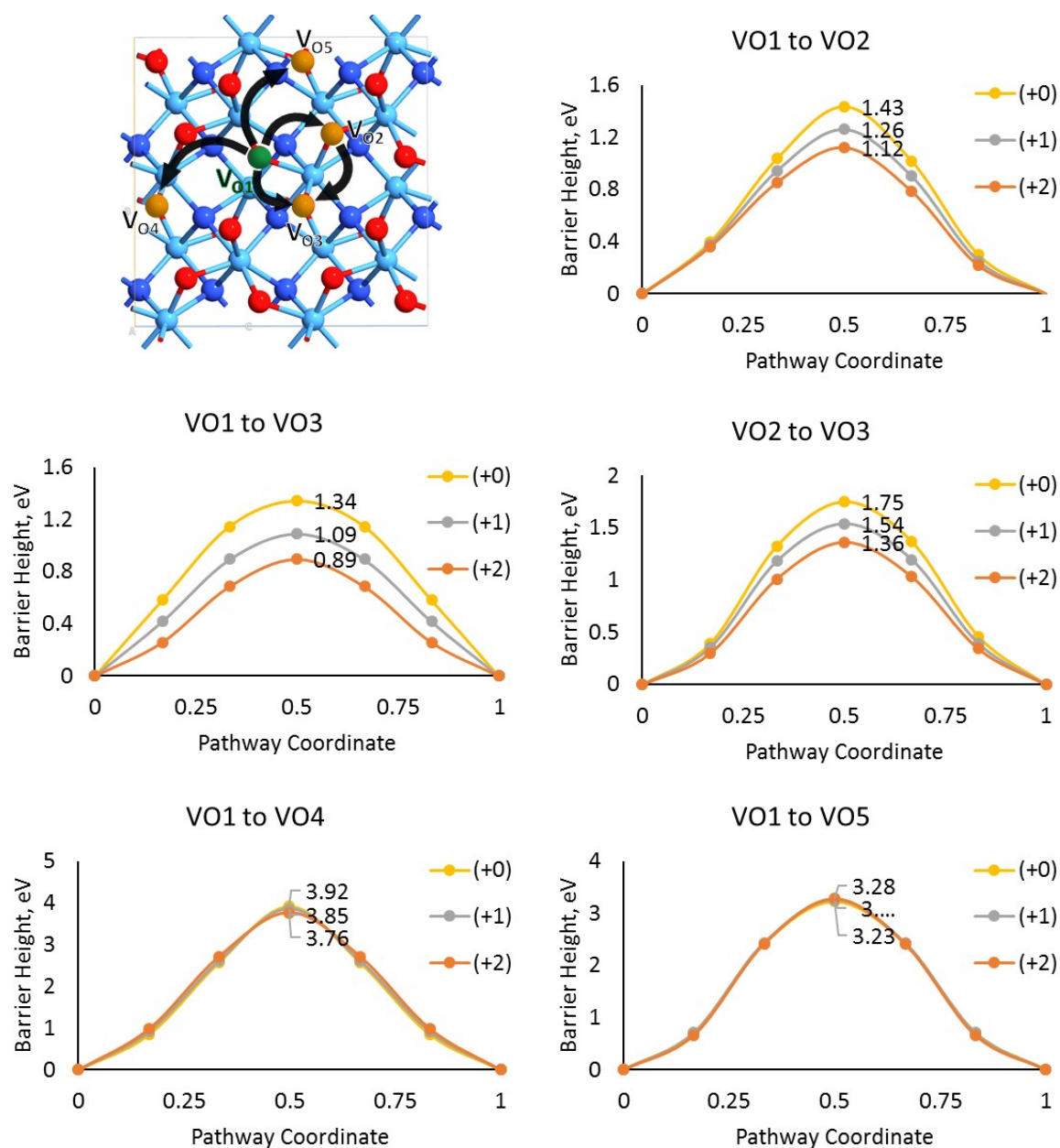


Figure S1. NEB Pathways corresponding to diffusion barriers reported in Figure 2.(a).

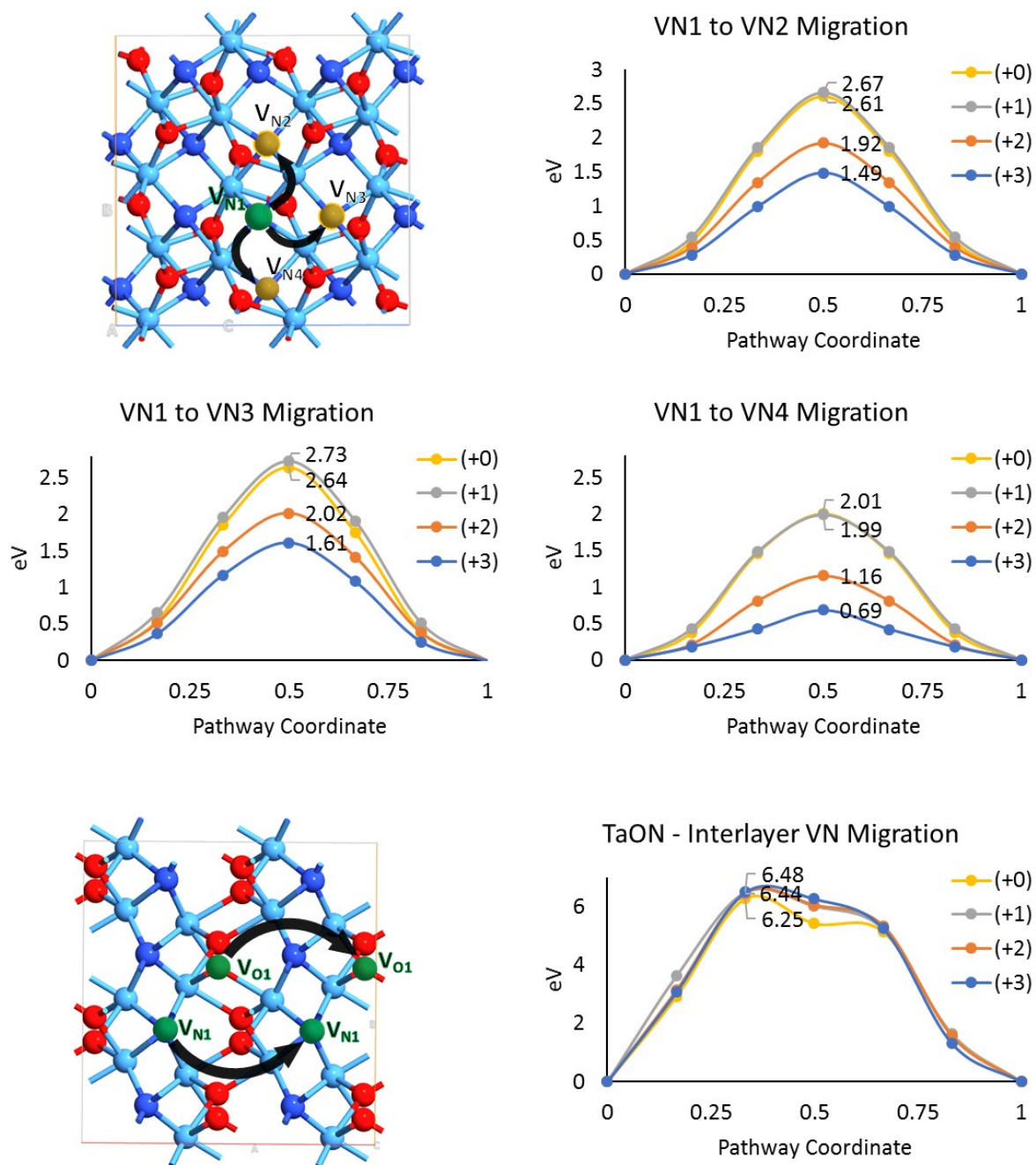


Figure S2. NEB Pathways corresponding to diffusion barriers reported in Figure 2.(b).

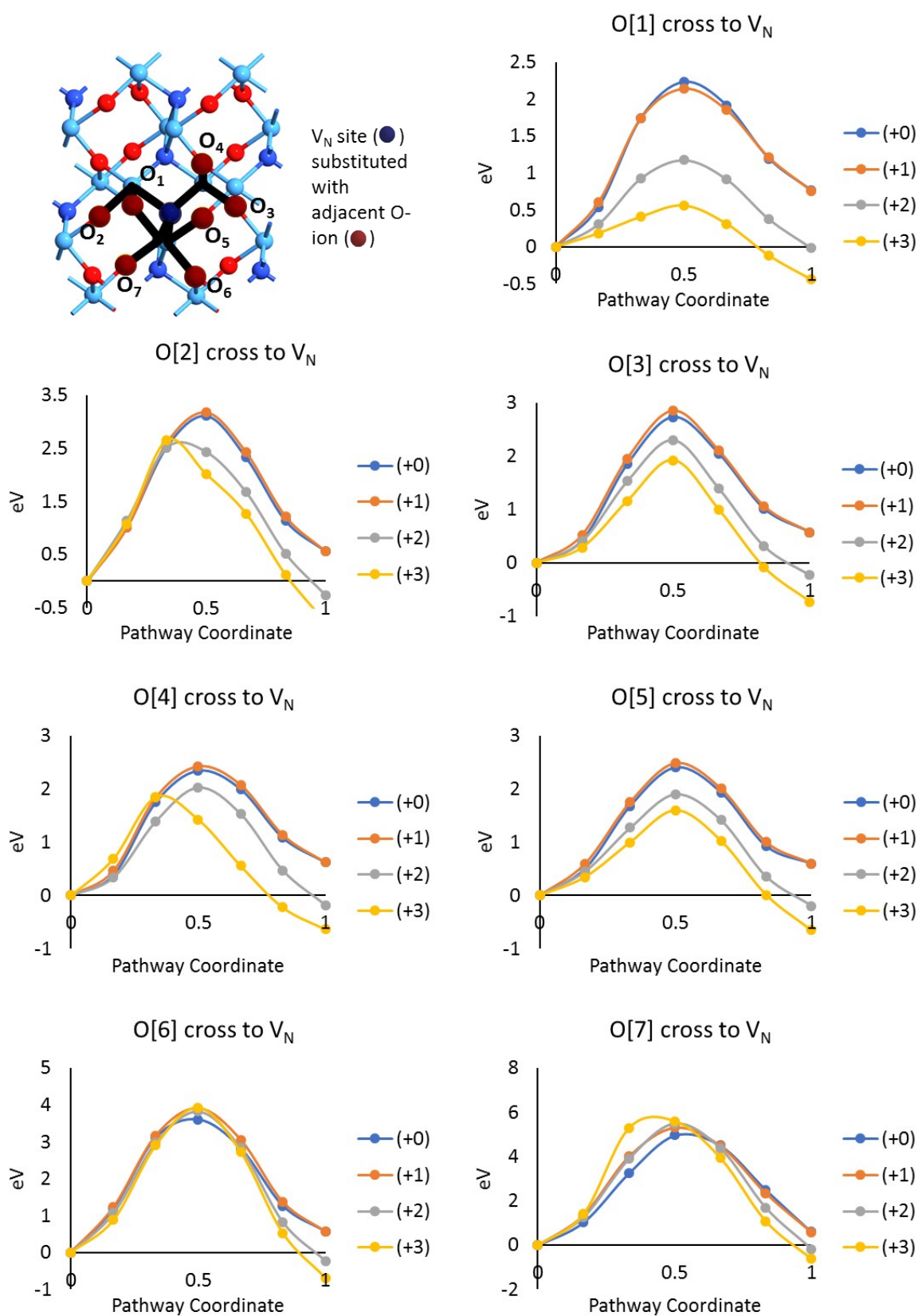


Figure S3. NEB Pathways corresponding to diffusion barriers reported in Figure 3.

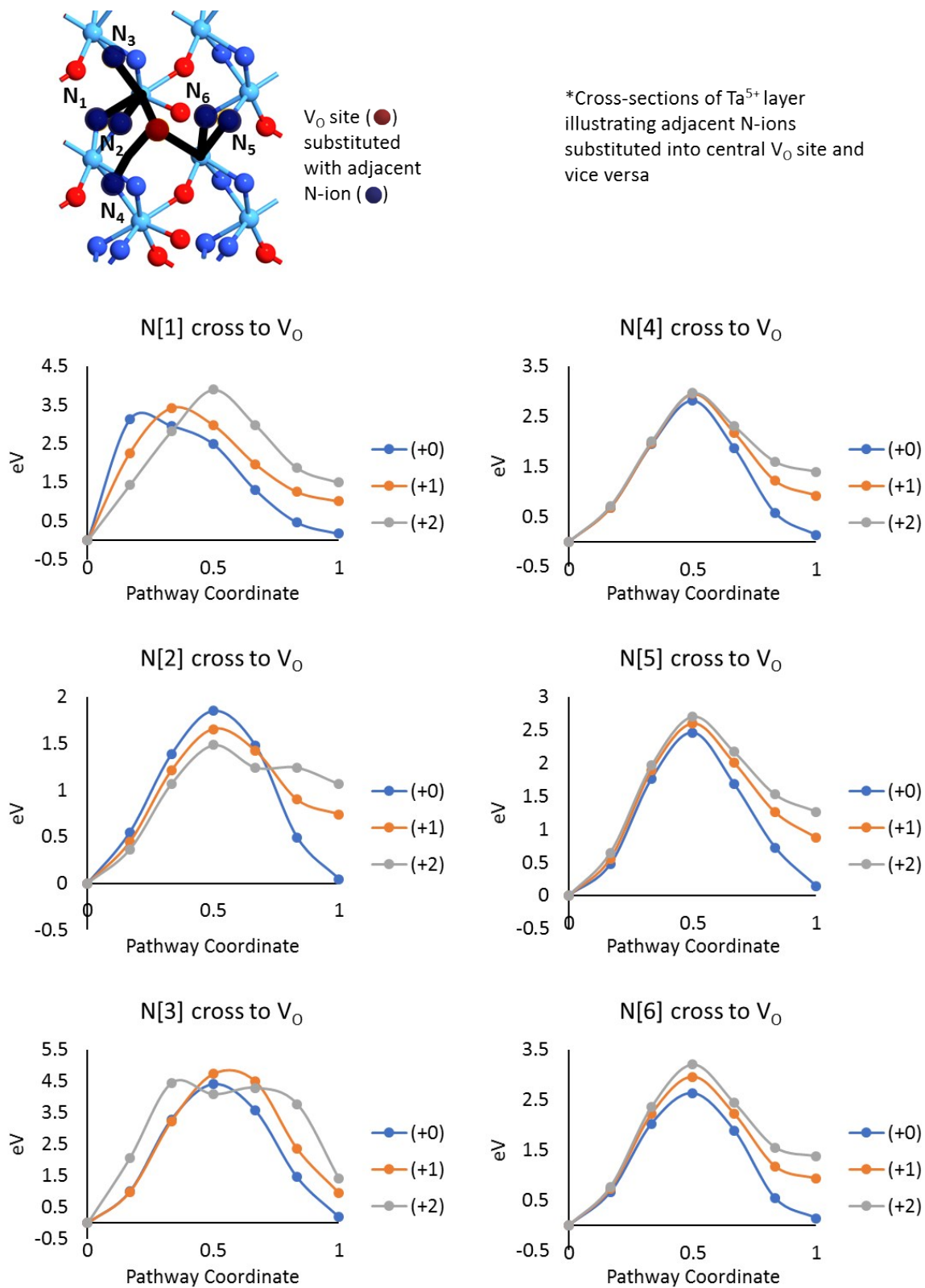
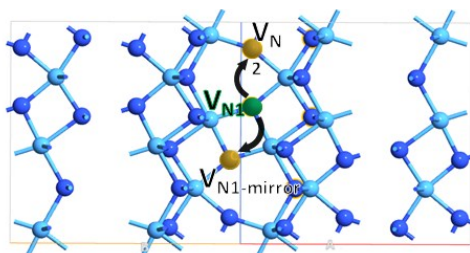
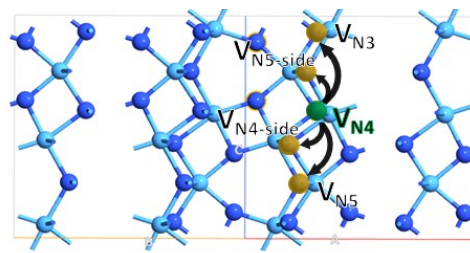
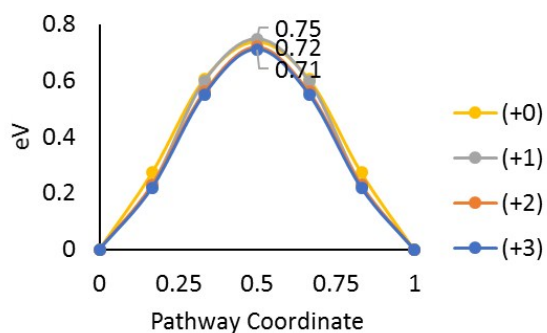


Figure S4. NEB Pathways corresponding to diffusion barriers reported in Figure 4.

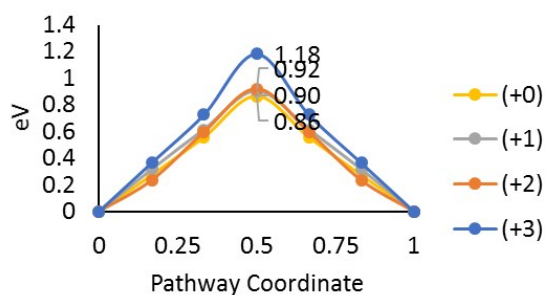


- between 3-coordinate N's

VN1a to VN1b

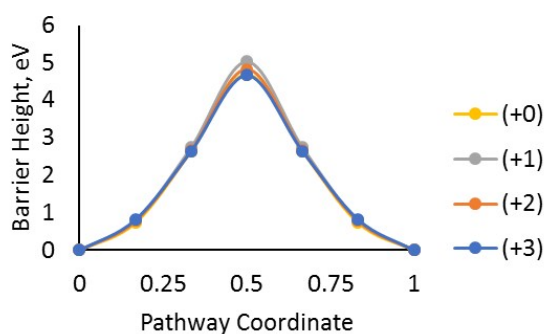


VN1 to VN2

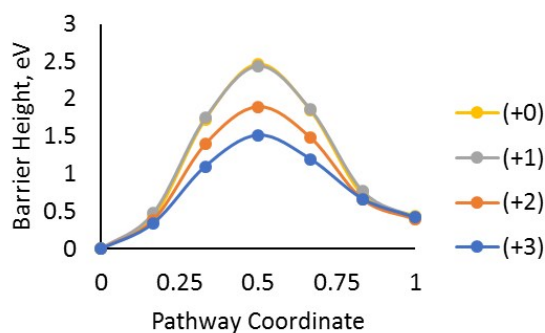


- between 4-coordinate N's

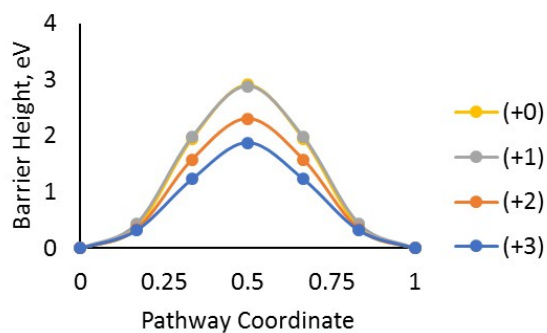
VN4 to VN3 Migration



VN4 to VN5-side



VN4 to VN4-side



VN4 to VN5

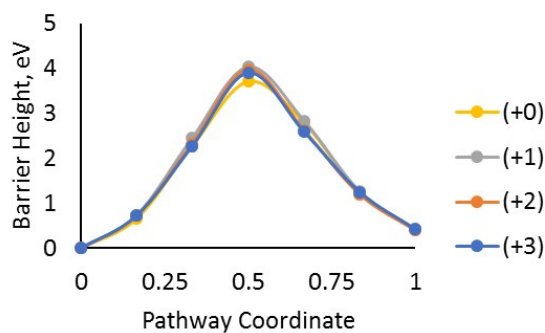


Figure S5. NEB Pathways corresponding to diffusion barriers reported in Figure 5.(a) &(b)

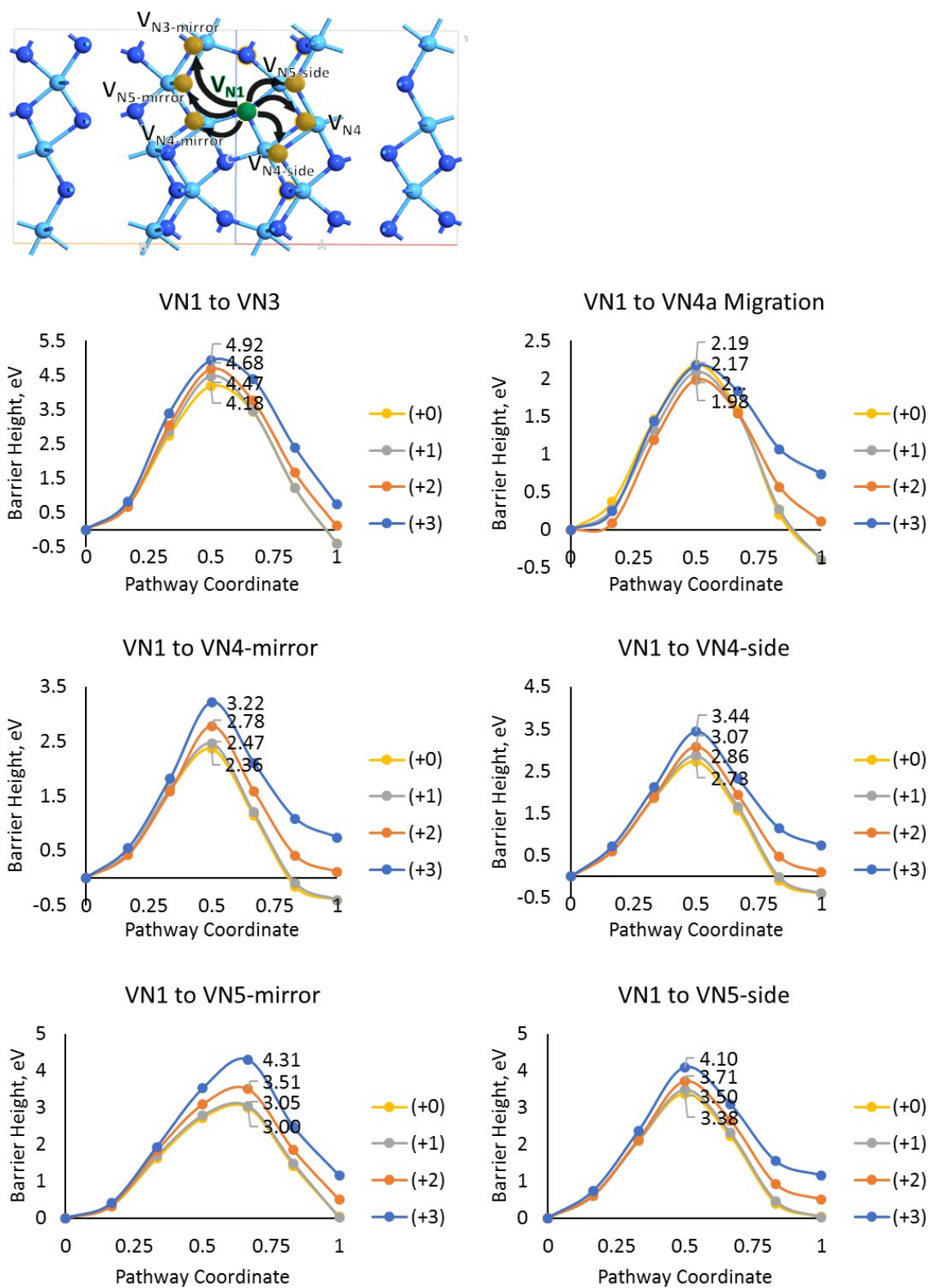
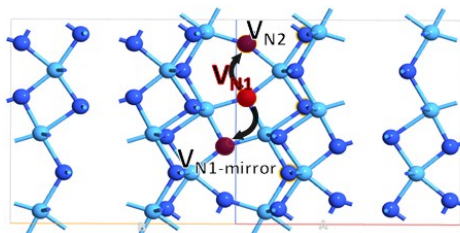
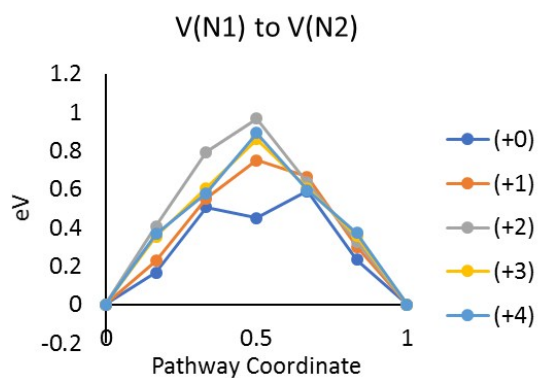
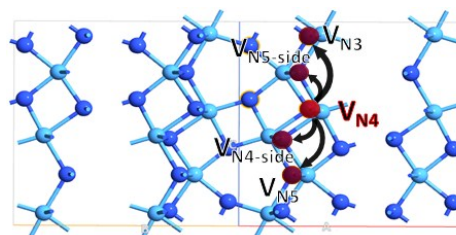
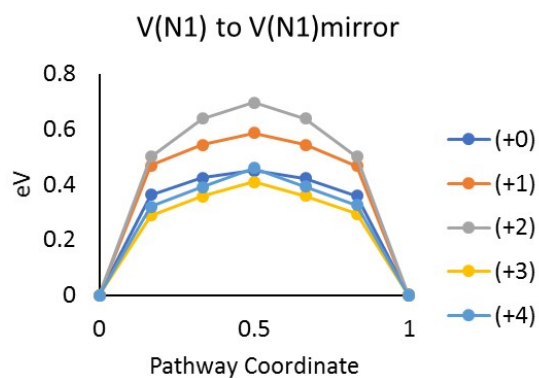


Figure S6. NEB Pathways corresponding to diffusion barriers reported in Figure 5.(c)



- between 3-coordinate N's



- between 4-coordinate N's

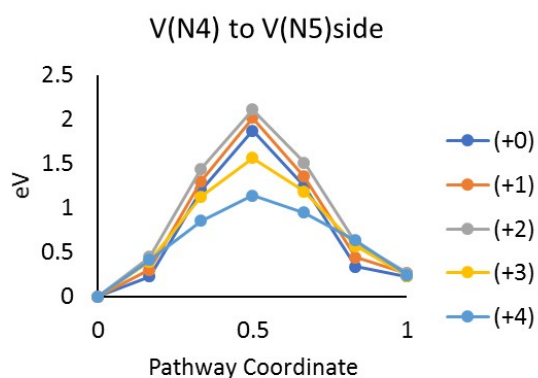
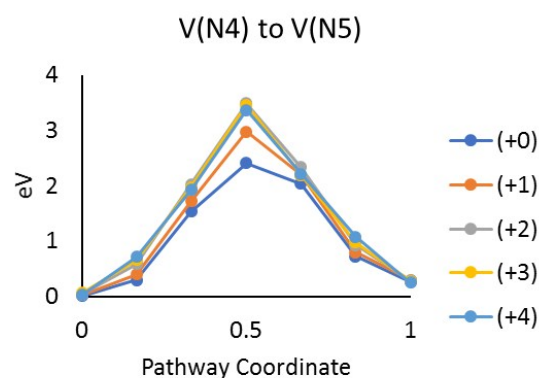
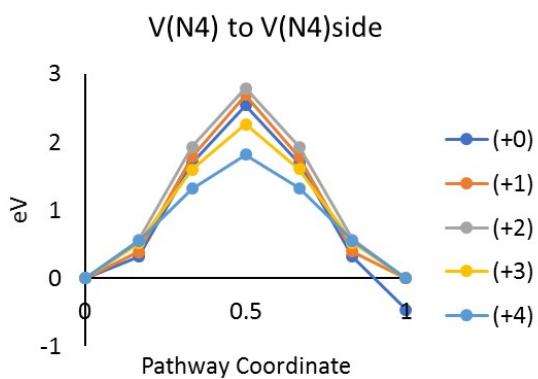
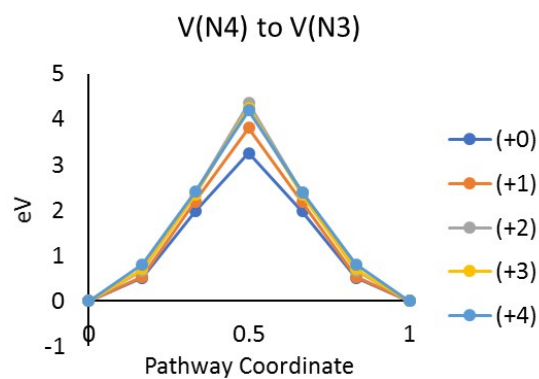


Figure S7. NEB Pathways corresponding to diffusion barriers reported in Figure 6.(a) &(b)

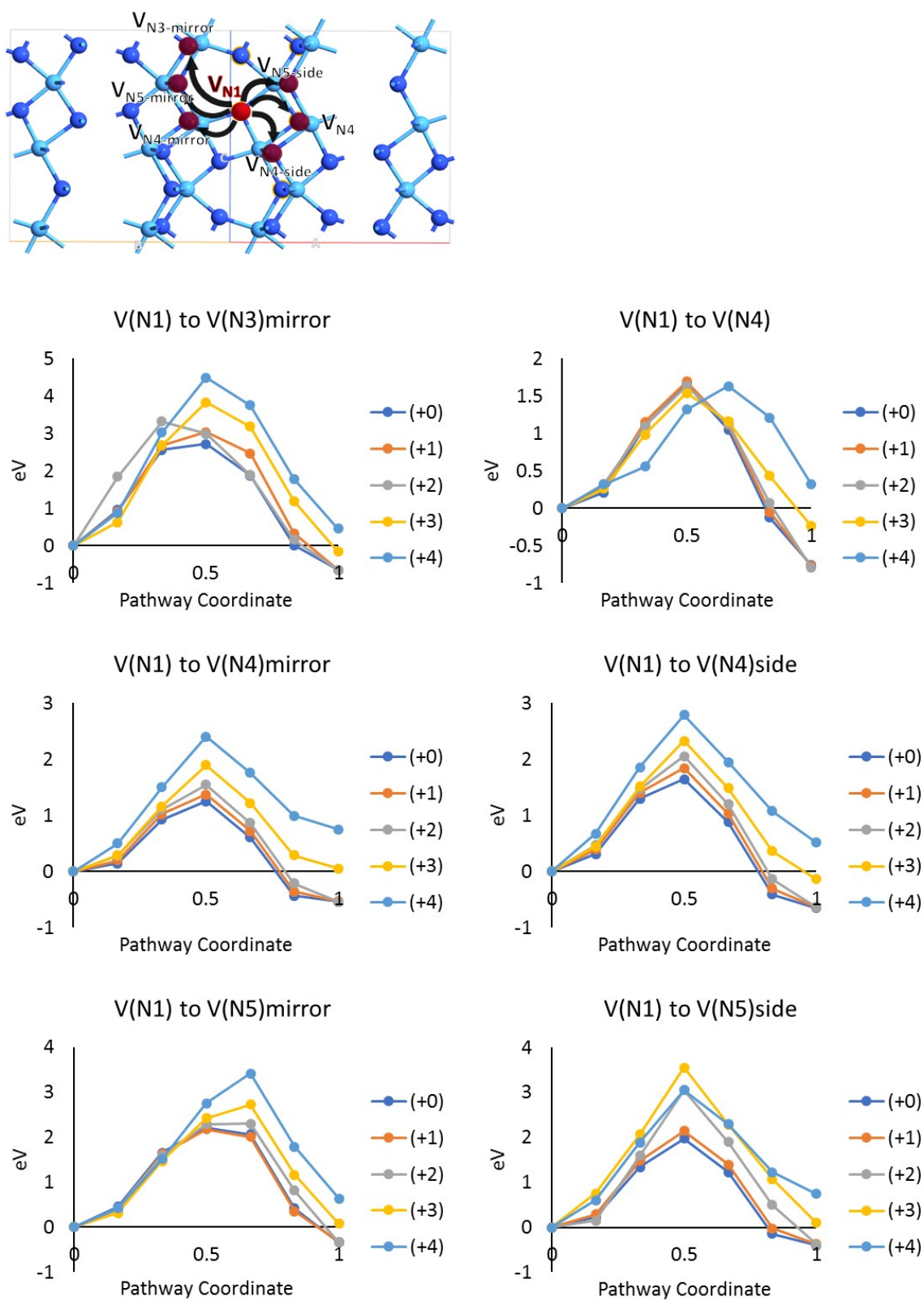


Figure S8. NEB Pathways corresponding to diffusion barriers reported in Figure 6.(c)