

Supplementary Material

Theoretical Study on the Effects of Alloying Elements on TiO₂/Ti₂AlNb Interface Adhesion Properties

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This Supplementary Material includes seven Supplementary Figures:

Figure S1. Convergence of cutoff energy and k-mesh

Figure S2. W_{sep} -distance curve and stress-strain curve of normal separation process of alloying elements doped TiO₂/Ti₂AlNb interface

Figure S3. W_{sep} -distance curve and stress-strain curve of tangential separation process of alloying elements doped TiO₂/Ti₂AlNb interface

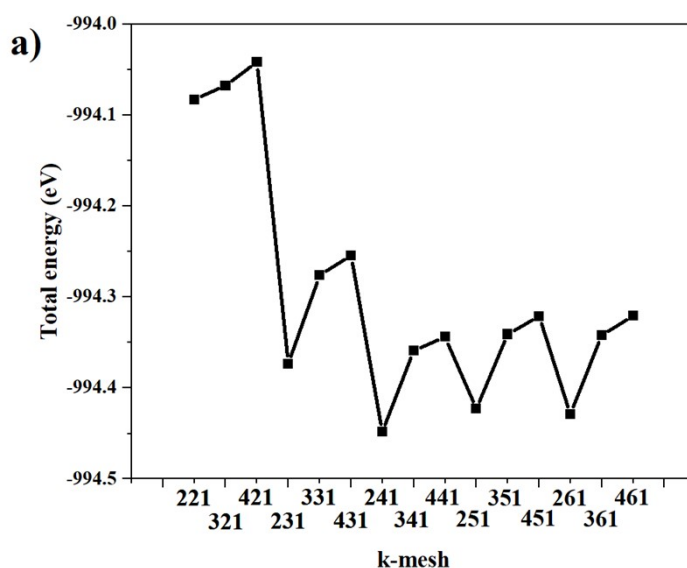
Figure S4. Differential charge densities of the bare TiO₂/Ti₂AlNb interface during normal separation

Figure S5. Differential charge densities of the Si element doped (Nb substituted) TiO₂/Ti₂AlNb interface during normal separation

Figure S6. Differential charge densities of the Hf element doped (Nb substituted) TiO₂/Ti₂AlNb interface during normal separation

Figure S7. The relaxation process of first-principles molecular dynamics

Figure S8. Structural changes of the TiO₂/Ti₂AlNb interface at 1100K



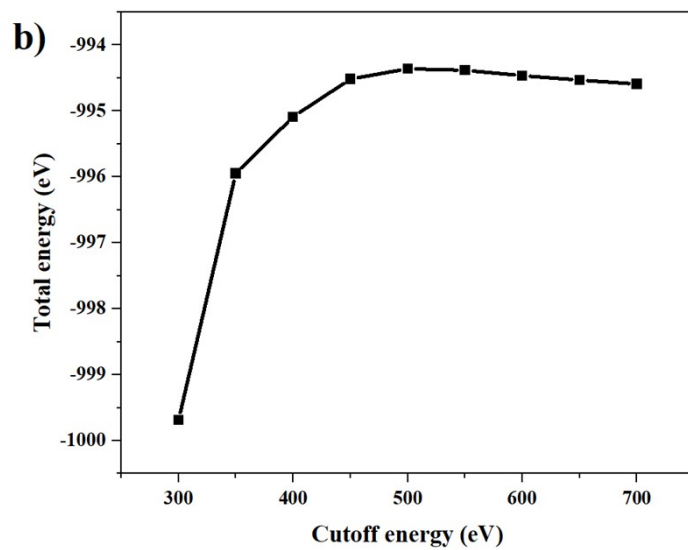
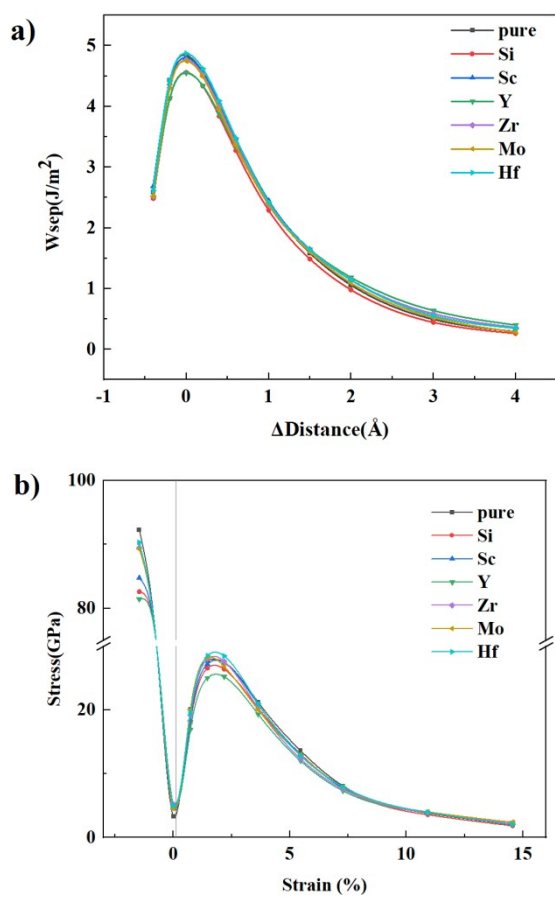


Fig. 1 Convergence of cutoff energy and k-mesh



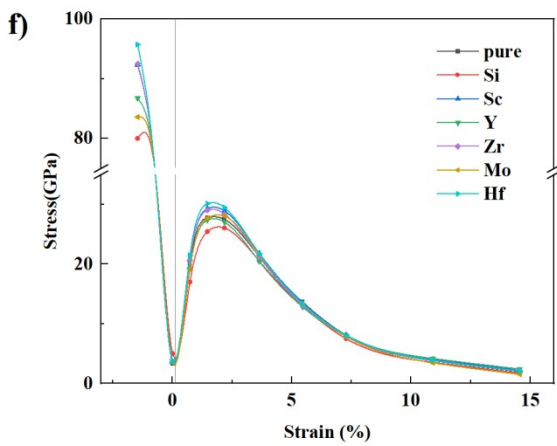
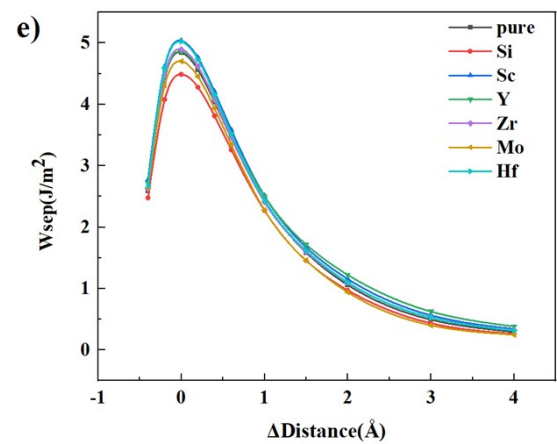
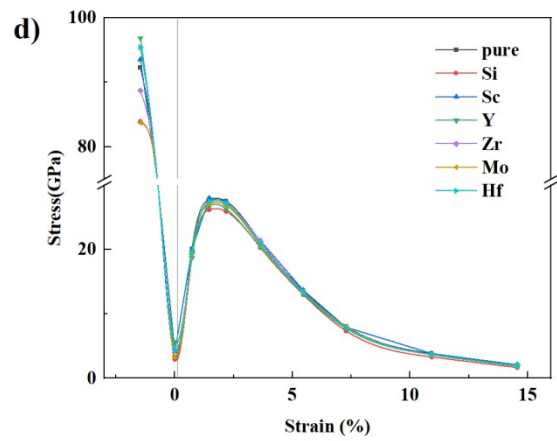
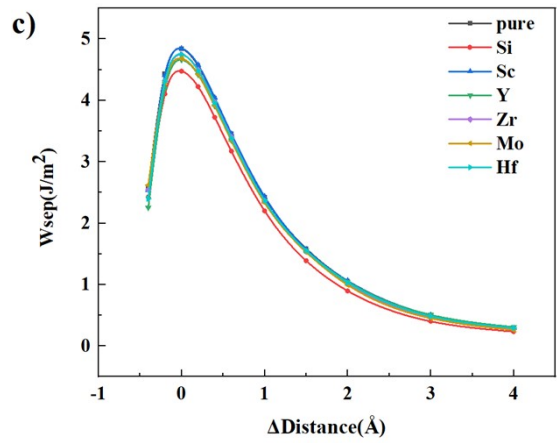
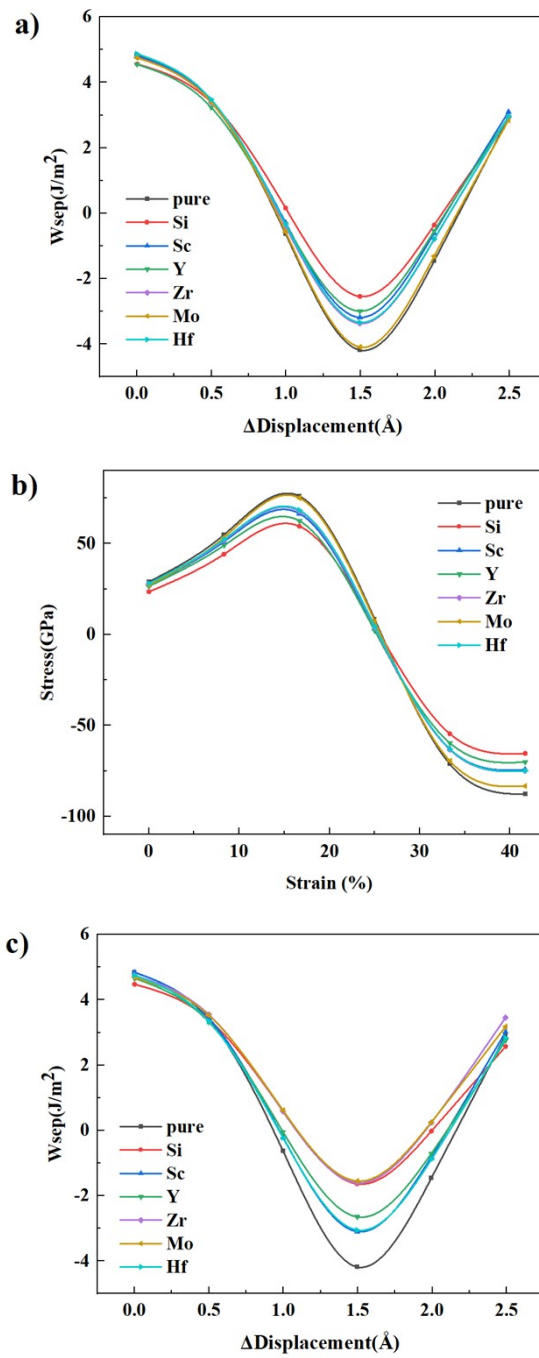


Fig. 2 a) W_{sep} -distance curve and b) stress-strain curve of normal separation process of alloying elements doped (Al substituted) $\text{TiO}_2/\text{Ti}_2\text{AlNb}$ interface, c) W_{sep} -distance curve and d) stress-strain curve of normal separation process of alloying elements doped (Ti substituted) $\text{TiO}_2/\text{Ti}_2\text{AlNb}$ interface, e) W_{sep} -distance curve and f) stress-strain curve of normal separation process of alloying elements doped (Nb substituted) $\text{TiO}_2/\text{Ti}_2\text{AlNb}$ interface



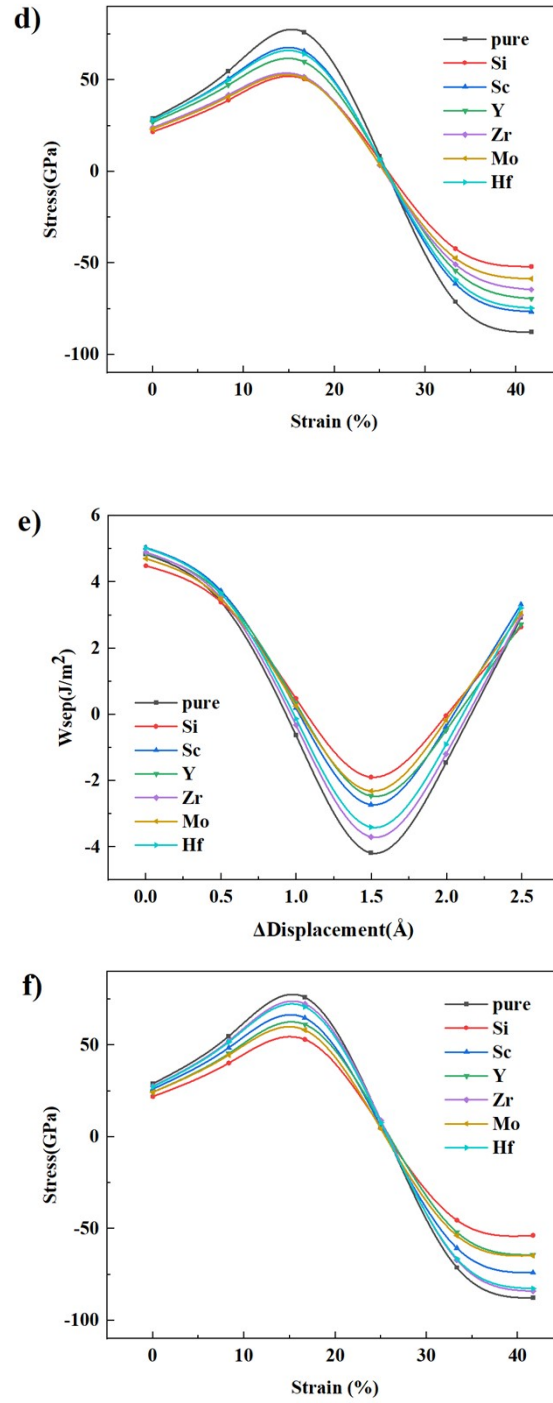


Fig. 3 a) W_{sep} -distance curve and b) stress-strain curve of tangential separation process of alloying elements doped (Al substituted) $\text{TiO}_2/\text{Ti}_2\text{AlNb}$ interface, c) W_{sep} -distance curve and d) stress-strain curve of tangential separation process of alloying elements doped (Ti substituted) $\text{TiO}_2/\text{Ti}_2\text{AlNb}$ interface, e) W_{sep} -distance curve and f) stress-strain curve of tangential separation process of alloying elements doped (Nb substituted) $\text{TiO}_2/\text{Ti}_2\text{AlNb}$ interface

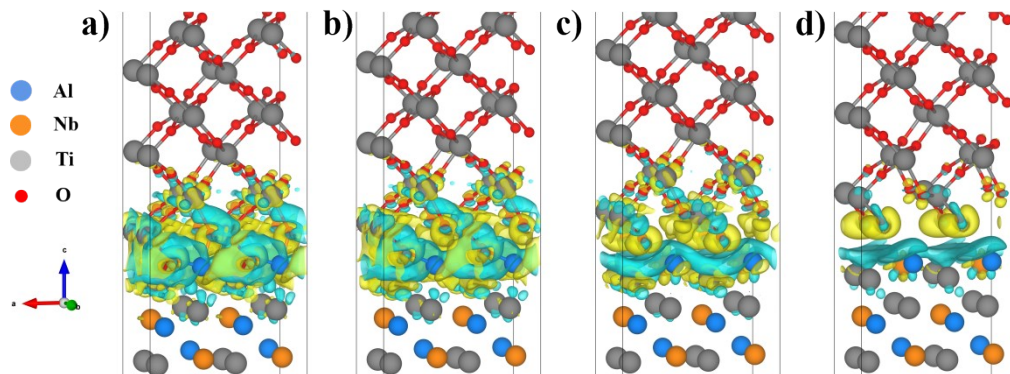


Fig. 4 Differential charge densities of the bare $\text{TiO}_2/\text{Ti}_2\text{AlNb}$ interface during normal separation, a) Strain value of 0%, b) Strain value of 1.46%, c) Strain value of 3.65%, d) Strain value of 7.3%

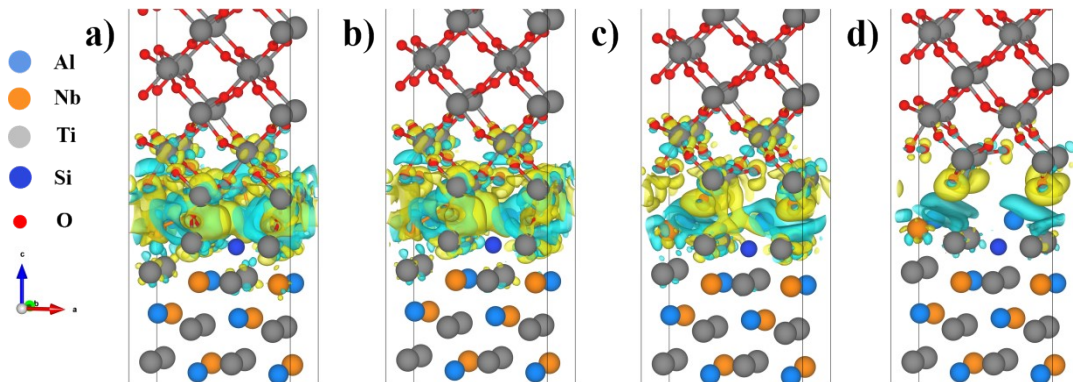


Fig. 5 Differential charge densities of the Si element doped (Nb substituted) $\text{TiO}_2/\text{Ti}_2\text{AlNb}$ interface during normal separation, a) Strain value of 0%, b) Strain value of 1.46%, c) Strain value of 3.65%, d) Strain value of 7.3%

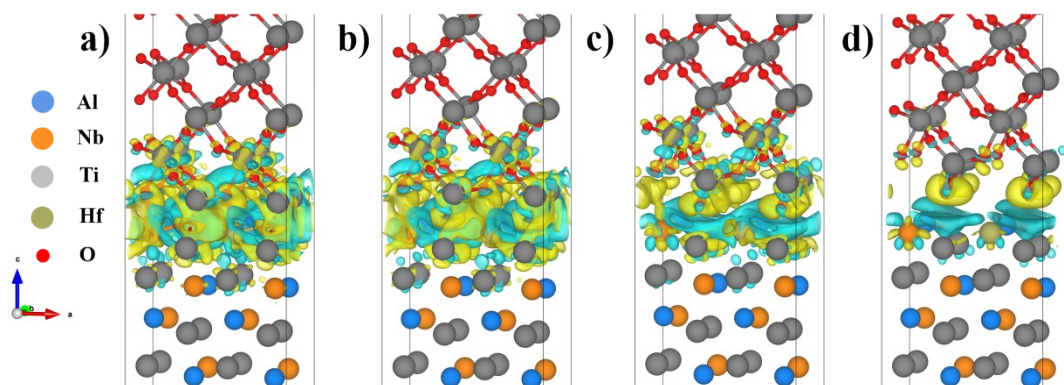
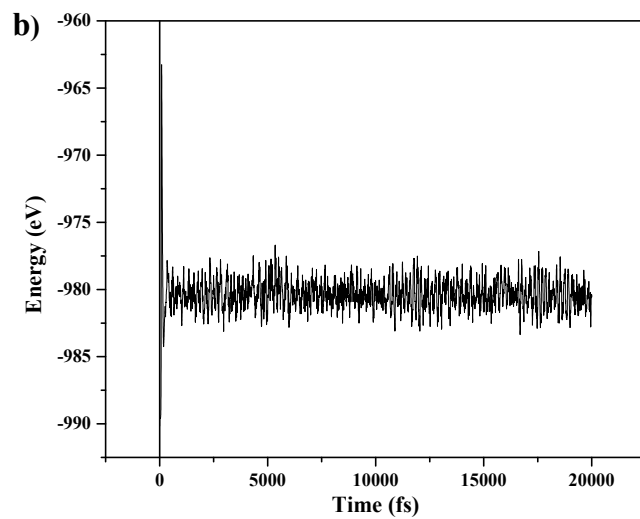
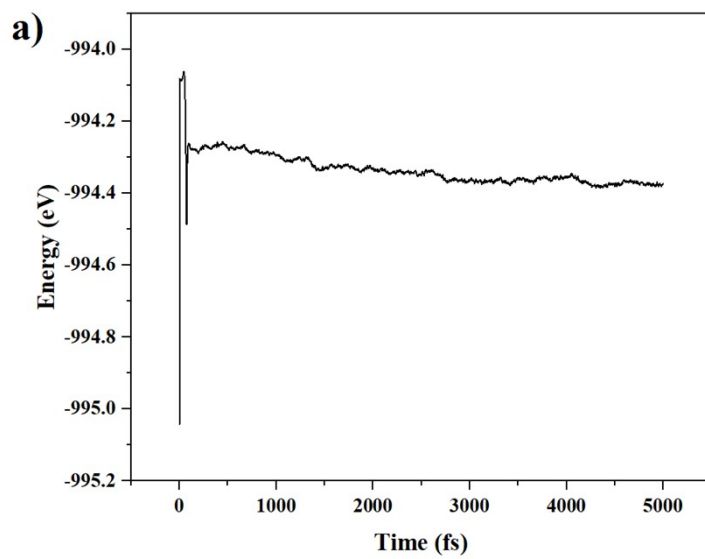


Fig. 6 Differential charge densities of the Hf element doped (Nb substituted) $\text{TiO}_2/\text{Ti}_2\text{AlNb}$ interface during normal separation, a) Strain value of 0%, b) Strain value of 1.46%, c) Strain value of 3.65%, d) Strain value of 7.3%



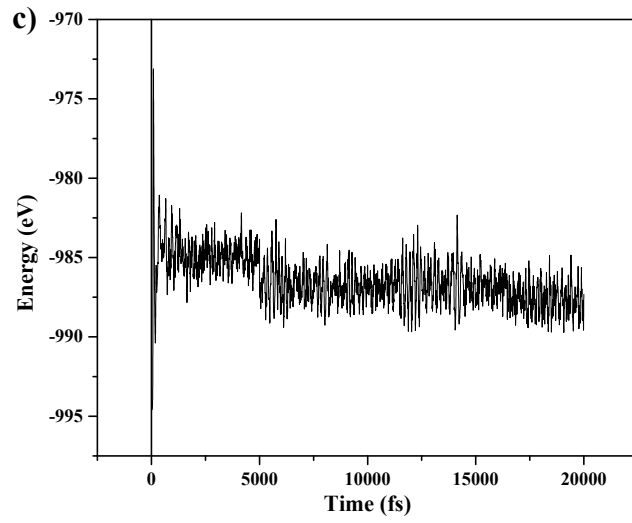


Fig. 7 The relaxation process of first-principles molecular dynamics, a) the bare $\text{TiO}_2/\text{Ti}_2\text{AlNb}$ interface, b) the Si doped $\text{TiO}_2/\text{Ti}_2\text{AlNb}$ interface, c) the Hf doped $\text{TiO}_2/\text{Ti}_2\text{AlNb}$ interface

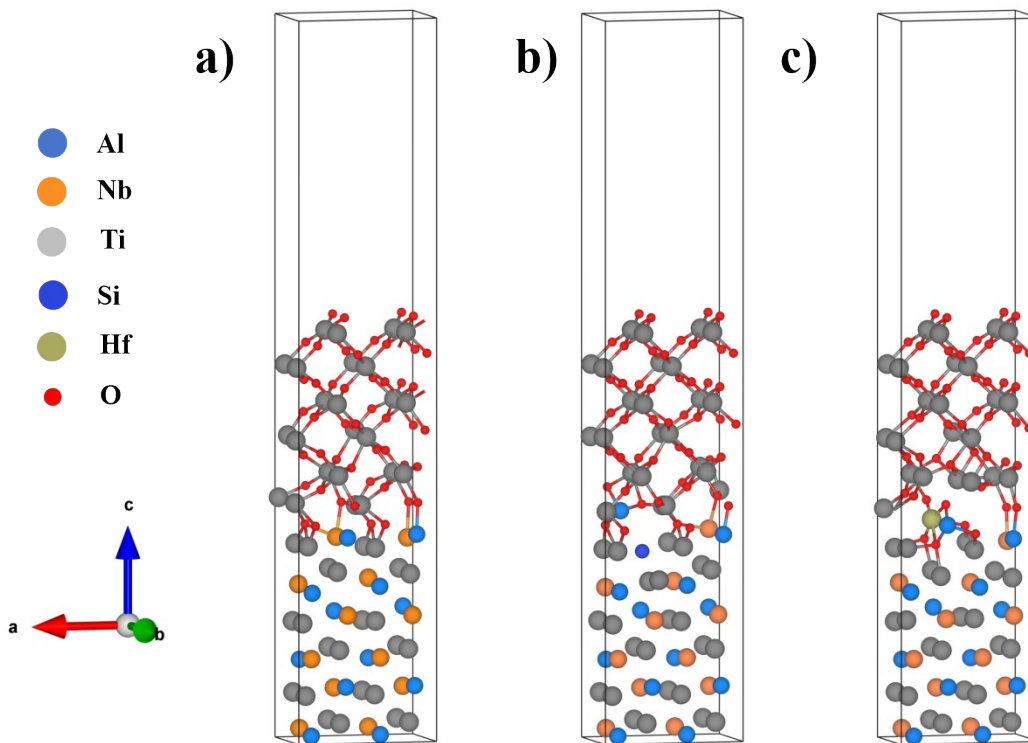


Fig. 8 Structural changes of the $\text{TiO}_2/\text{Ti}_2\text{AlNb}$ interface at 1100K, a) the bare $\text{TiO}_2/\text{Ti}_2\text{AlNb}$ interface, b) the Si doped $\text{TiO}_2/\text{Ti}_2\text{AlNb}$ interface, c) the Hf doped $\text{TiO}_2/\text{Ti}_2\text{AlNb}$ interface