

Electronic Supplementary Information (ESI)

Molecular insights into adhesive mechanisms of phosphate-based dental adhesives on zirconia surfaces: effects of zirconia crystal structure

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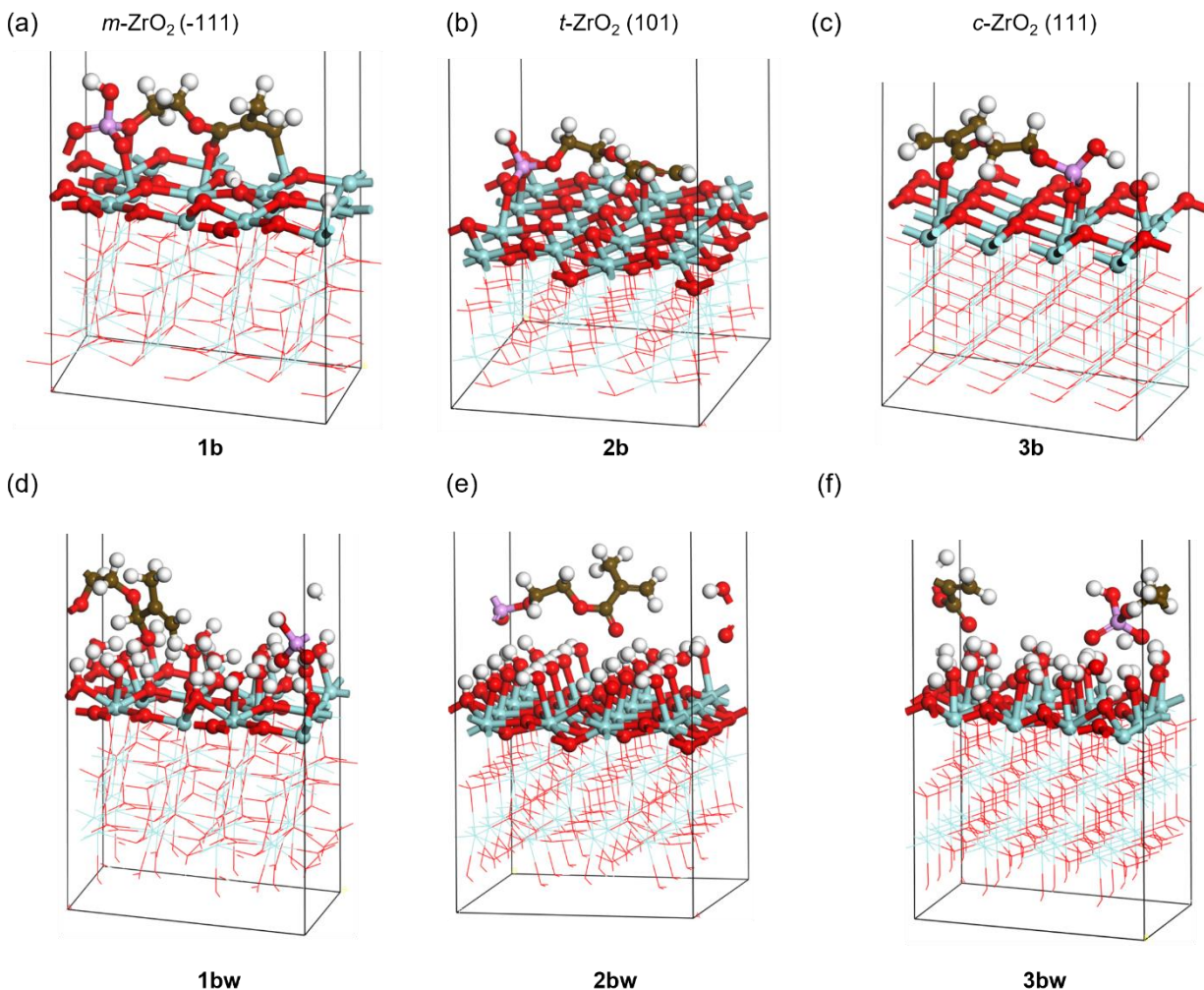


Fig. S1 Fixed atoms in density functional theory (DFT) optimizations. Atoms represented by thin lines are fixed and atoms represented by ball & stick are relaxed. (a) $m\text{-ZrO}_2(101)$, (b) $t\text{-ZrO}_2(-111)$, (c) $c\text{-ZrO}_2(111)$ surfaces. (d)-(f) are hydroxylated surfaces of (a)-(c).