# Supporting Information for

# Cooperative Roles of Chemical Reactions and Mechanical Friction in Chemical Mechanical Polishing of Gallium Nitride Assisted by OH Radicals: Tight-Binding Quantum Chemical Molecular Dynamics Simulations

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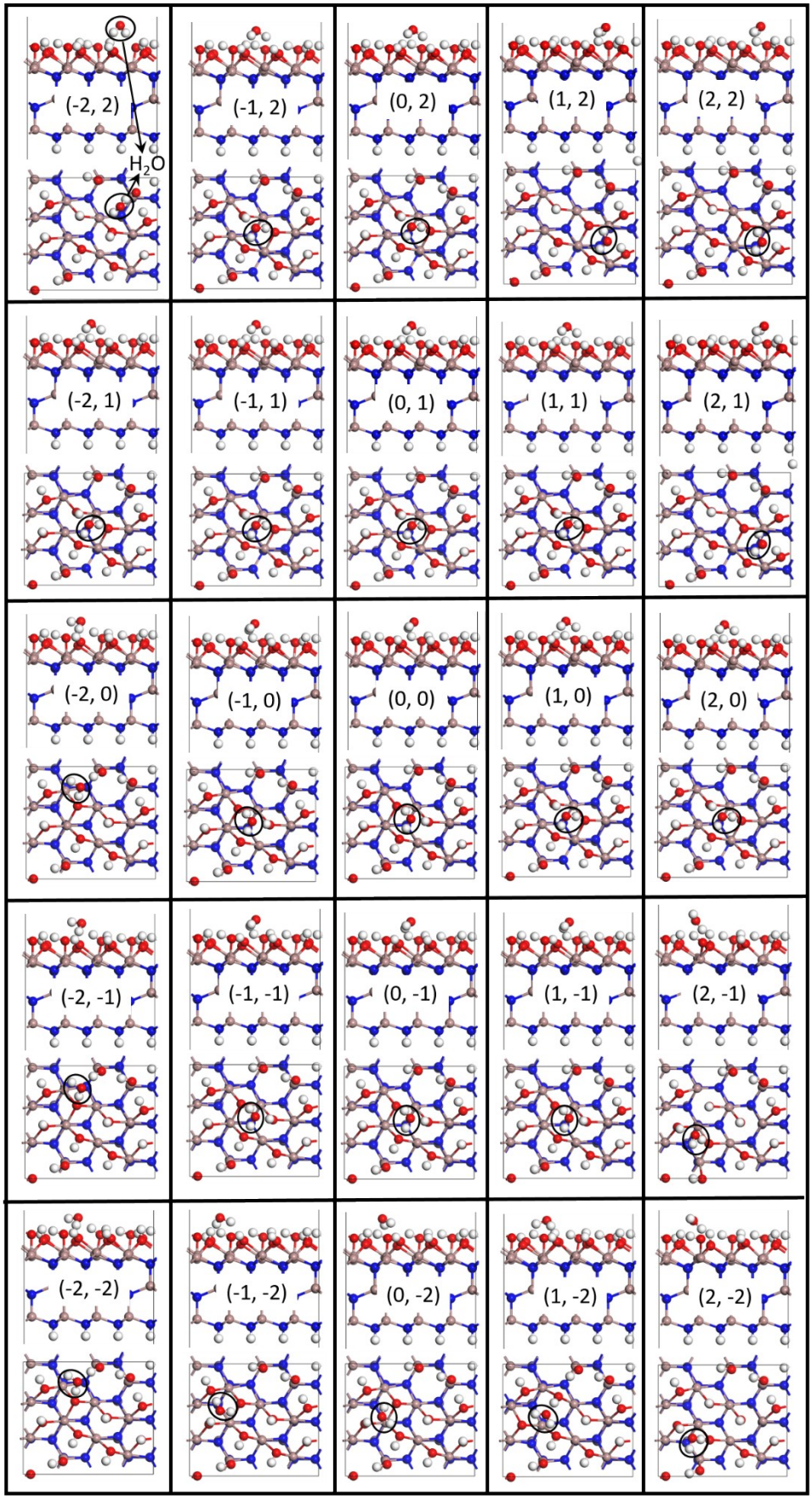
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**Figure S1.** Post-optimized structure of GaN substrate structures of GaN substrate with 25 different initial positions of OH radical. The model of GaN substrate is the same as that in Figure 8 of manuscript, while the *x*- and *y*-positions of the OH radical are varied. In details, the positions of OH radical in Figure 8 is set as a datum point, and $(i, j)$ indicates that the OH radical is moved with $i$ Å along *x*-direction and $j$ Å along *y*-direction from the datum point. For all calculations, front view and top view are given.