Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Mechanism of Wettability Alteration of the Calcite {$10\bar{1}4$} Surface

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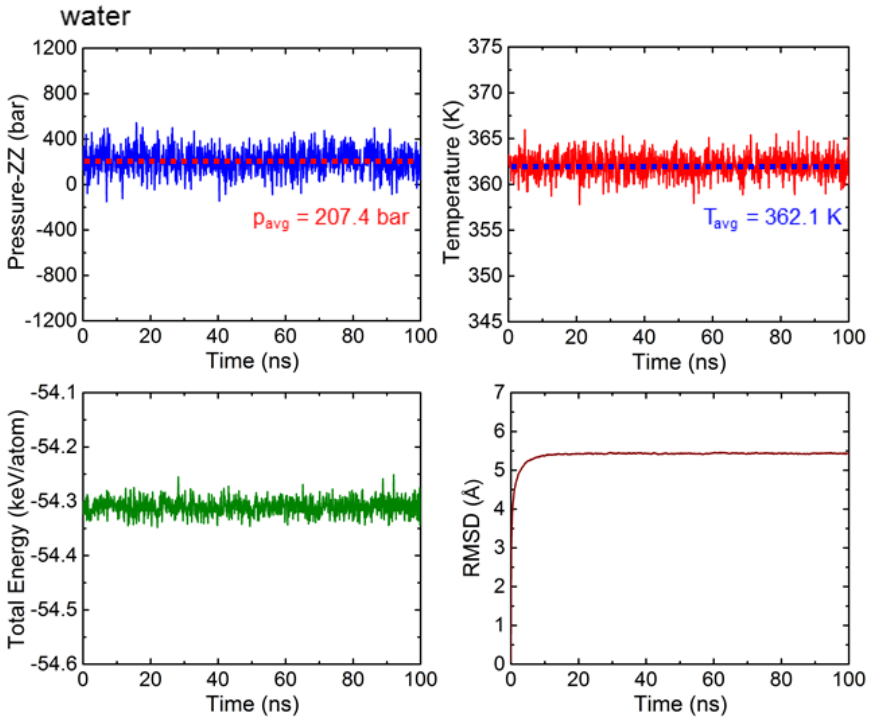

Figure S1. Pressure, temperature, total energy, and root mean square deviation in the NPT MD simulation of (deionized) water on the calcite $\{10\bar{1}4\}$ surface.

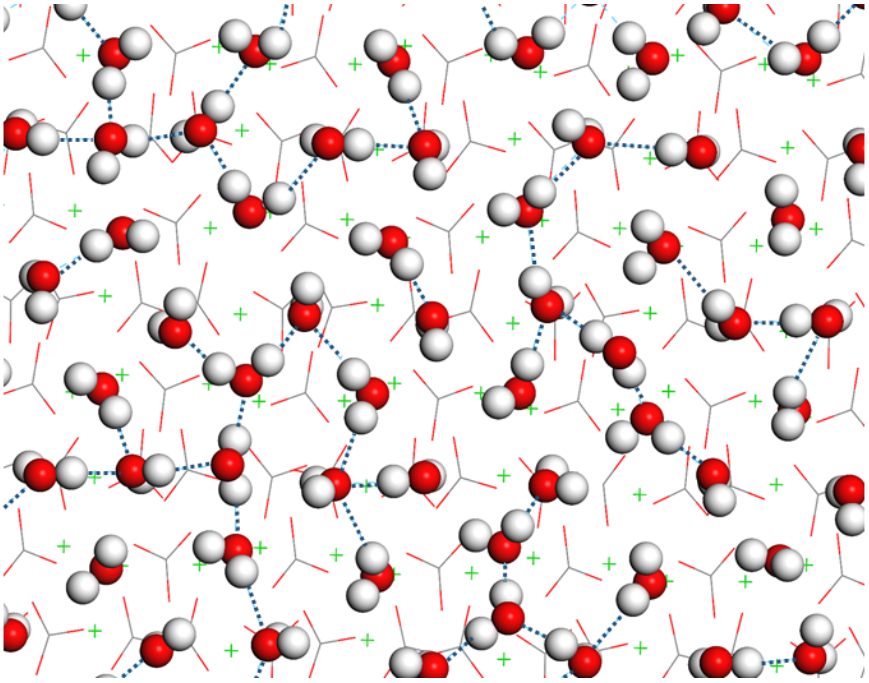

Figure S2. Arrangement of water molecules on the calcite $\{10\bar{1}4\}$ surface (average structure from the last 5 ps of the MD simulation). H is represented in white and O in red.

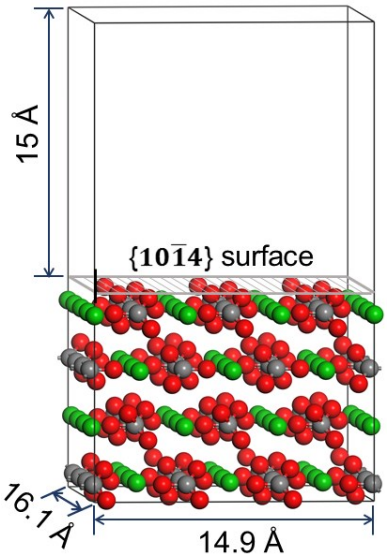

Figure S3. Side view of the calcite slab used in the simulations (2 × 3 supercell, four layers of Ca^{2+} and CO_3^{2-} ions; vacuum region of 15 Å thickness). C is represented in gray, O in red, and Ca in green.

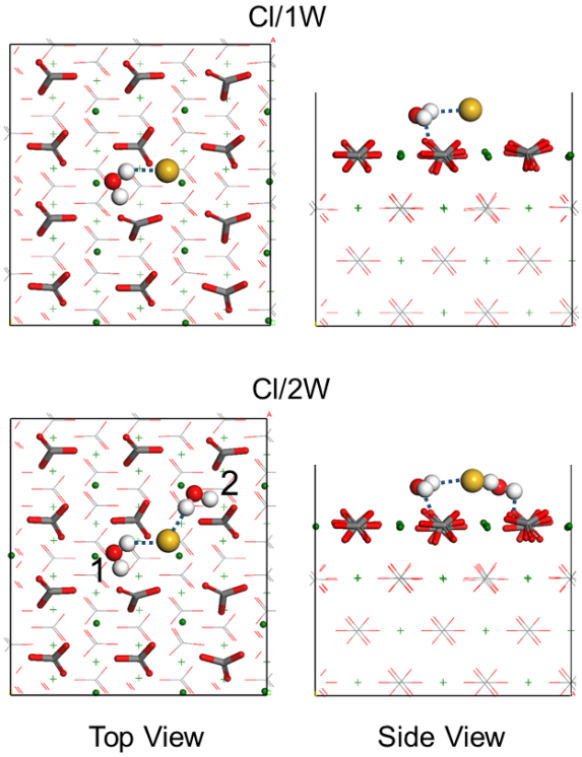

Figure S4. Top and side views of the favorable binding geometries of one Cl^- ion and one (1W) or two (2W) water molecules (numbered) on the calcite {10$\bar{1}$4} surface. Dashed lines mark hydrogen bonds. H is represented in white, C in gray, O in red, Cl in gold, and Ca in green.

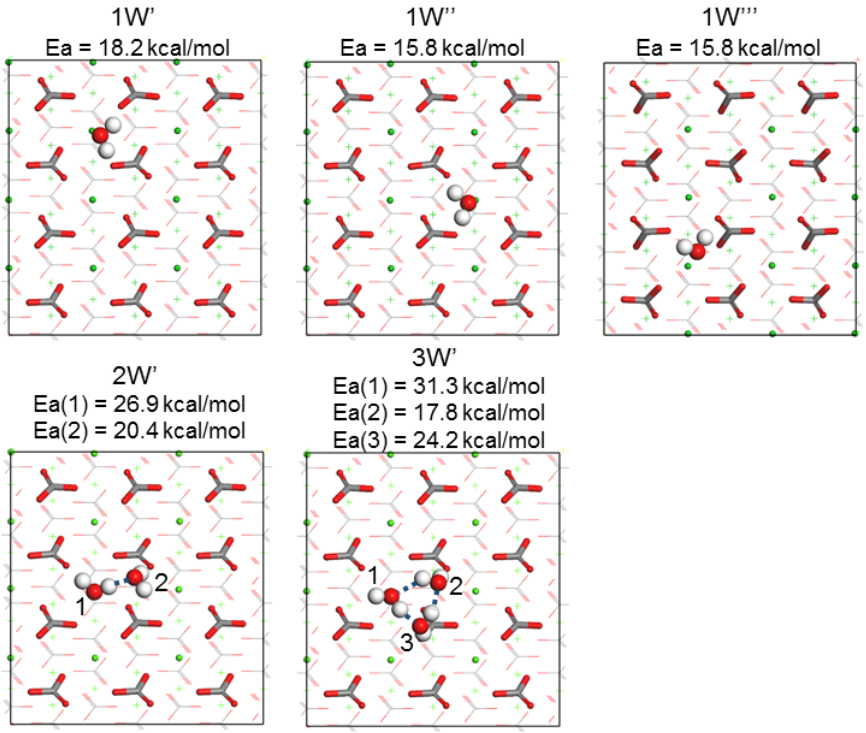

Figure S5. Top views of the less favorable binding geometries for one (1W), two (2W), or three (3W) water molecules (numbered) on the calcite $\{10\bar{1}4\}$ surface. Dashed lines mark hydrogen bonds. H is represented in white, C in gray, O in red, and Ca in green.

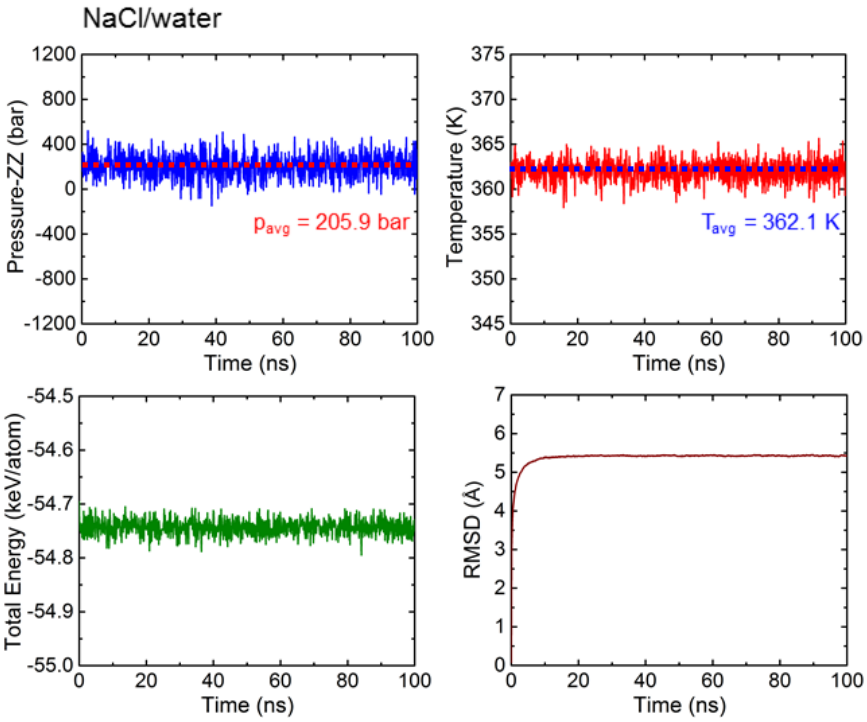

Figure S6. Pressure, temperature, total energy, and root mean square deviation in the NPT MD simulation of NaCl/water on the calcite $\{10\bar{1}4\}$ surface.

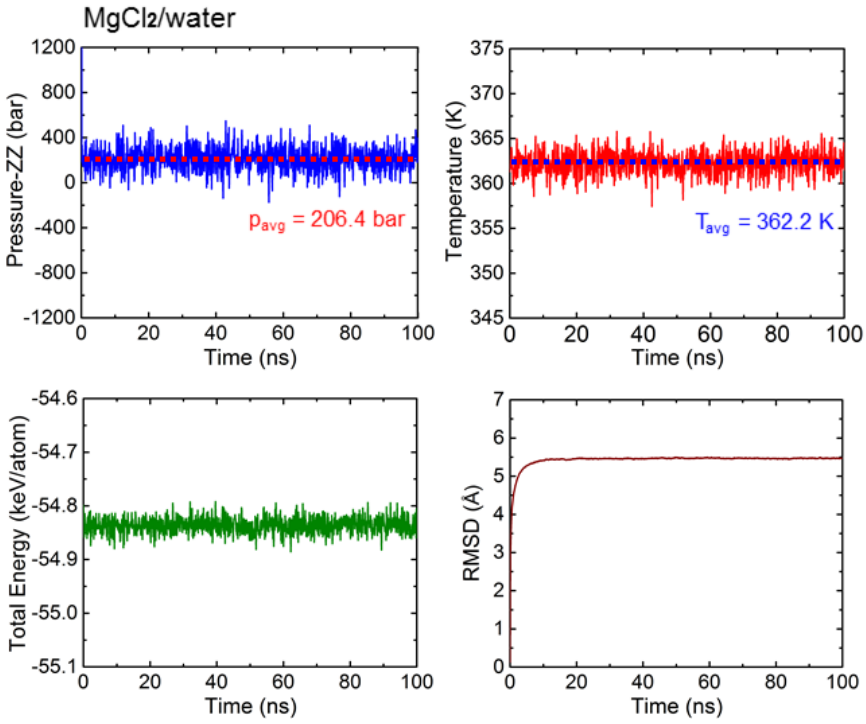

Figure S7. Pressure, temperature, total energy, and root mean square deviation in the NPT MD simulation of $MgCl_2$/water on the calcite $\{10\bar{1}4\}$ surface.

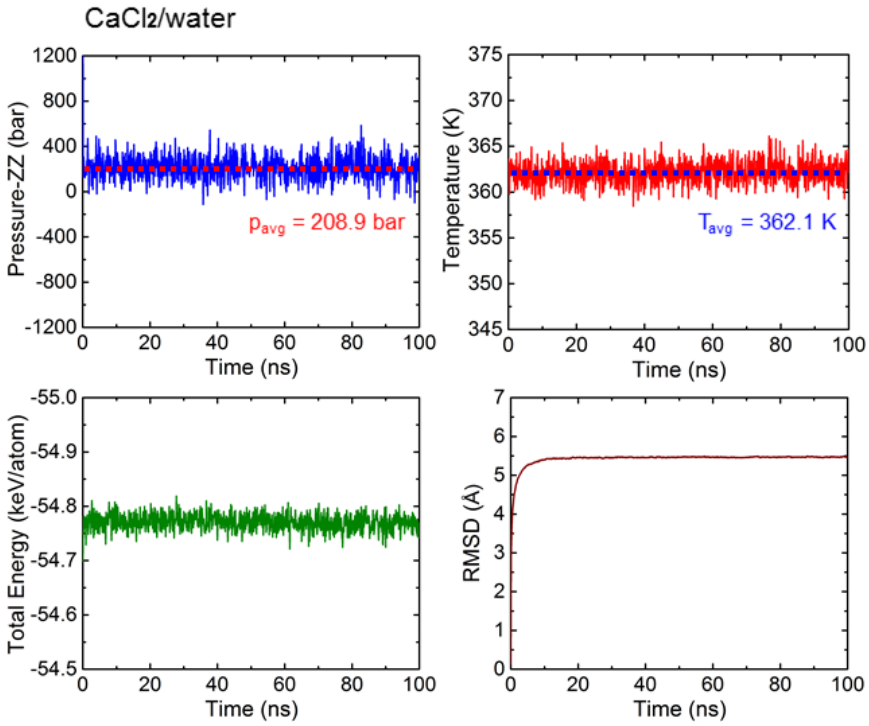

Figure S8. Pressure, temperature, total energy, and root mean square deviation in the NPT MD simulation of $CaCl_2$/water on the calcite $\{10\bar{1}4\}$ surface.

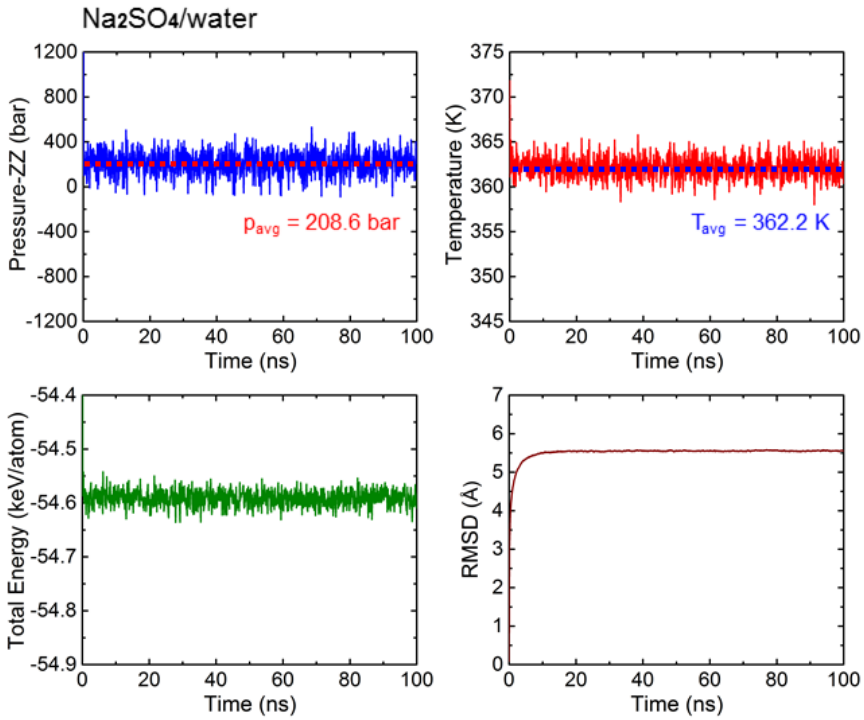

Figure S9. Pressure, temperature, total energy, and root mean square deviation in the NPT MD simulation of Na_2SO_4/water on the calcite $\{10\bar{1}4\}$ surface.

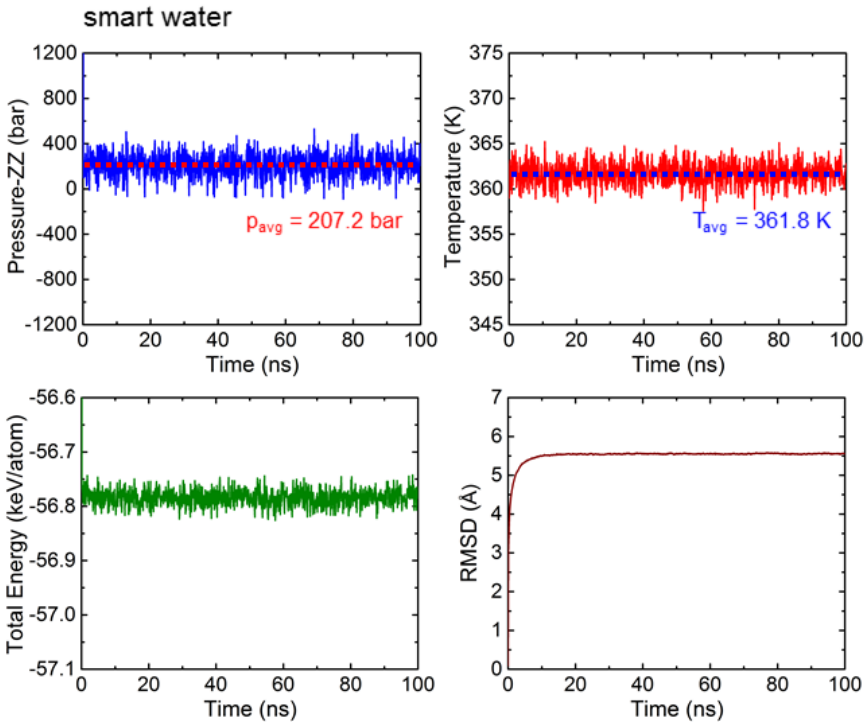

Figure S10. Pressure, temperature, total energy, and root mean square deviation in the NPT MD simulation of smart water on the calcite $\{10\bar{1}4\}$ surface.

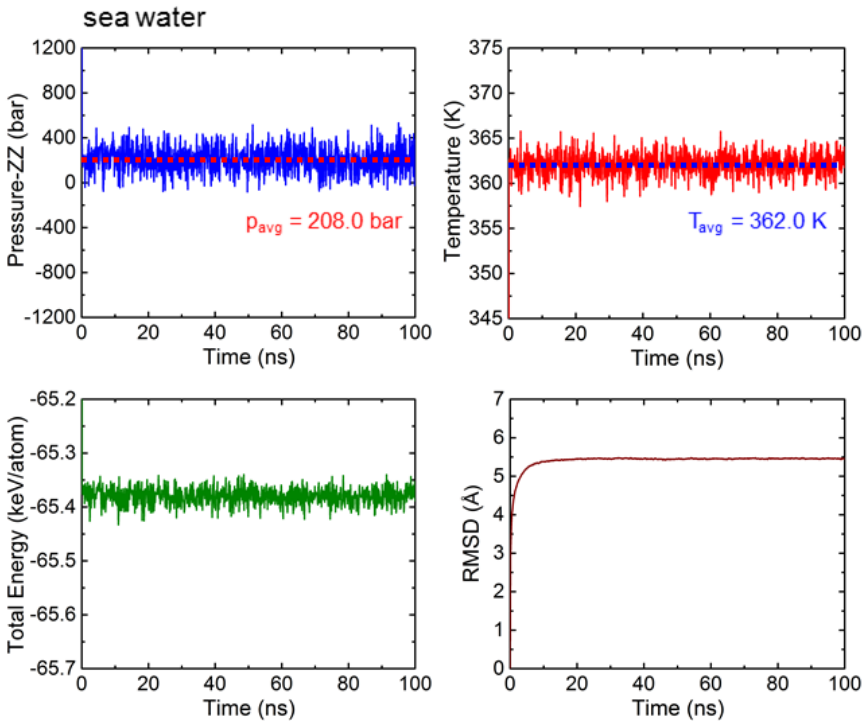

Figure S11. Pressure, temperature, total energy, and root mean square deviation in the NPT MD simulation of sea water on the calcite $\{10\bar{1}4\}$ surface.

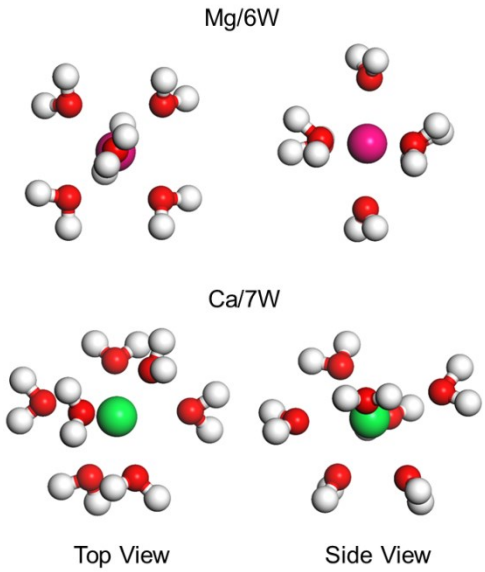

Figure S12. Representative structures of hydrated divalent salt ions ($Mg^{2+}\cdot 6H_2O$, $Ca^{2+}\cdot 7H_2O$; average structure from the last 5 ps of the MD simulation). H is represented in white, O in red, Ca in green, and Mg in magenta.

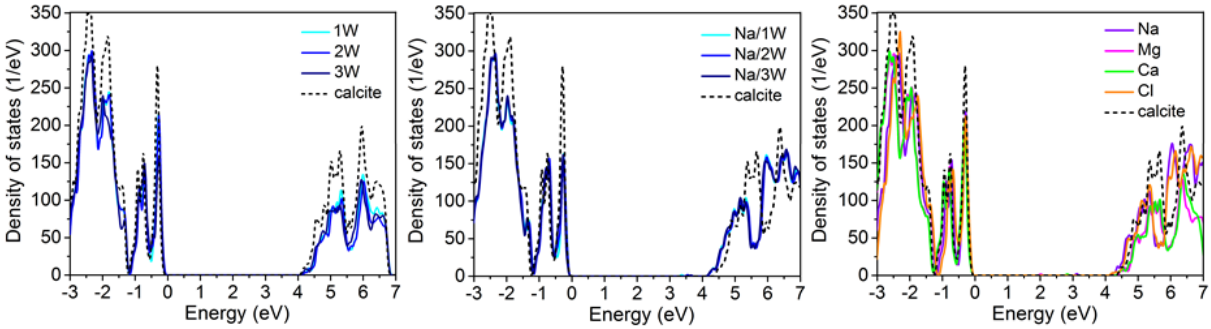

Figure S13. Effect of the charge transfer reported in Table 3 on the density of states.