

Supplementary Material

Termination Effects in Aluminosilicate and Aluminogermanate Imogolite Nanotubes: a Density Functional Theory Study

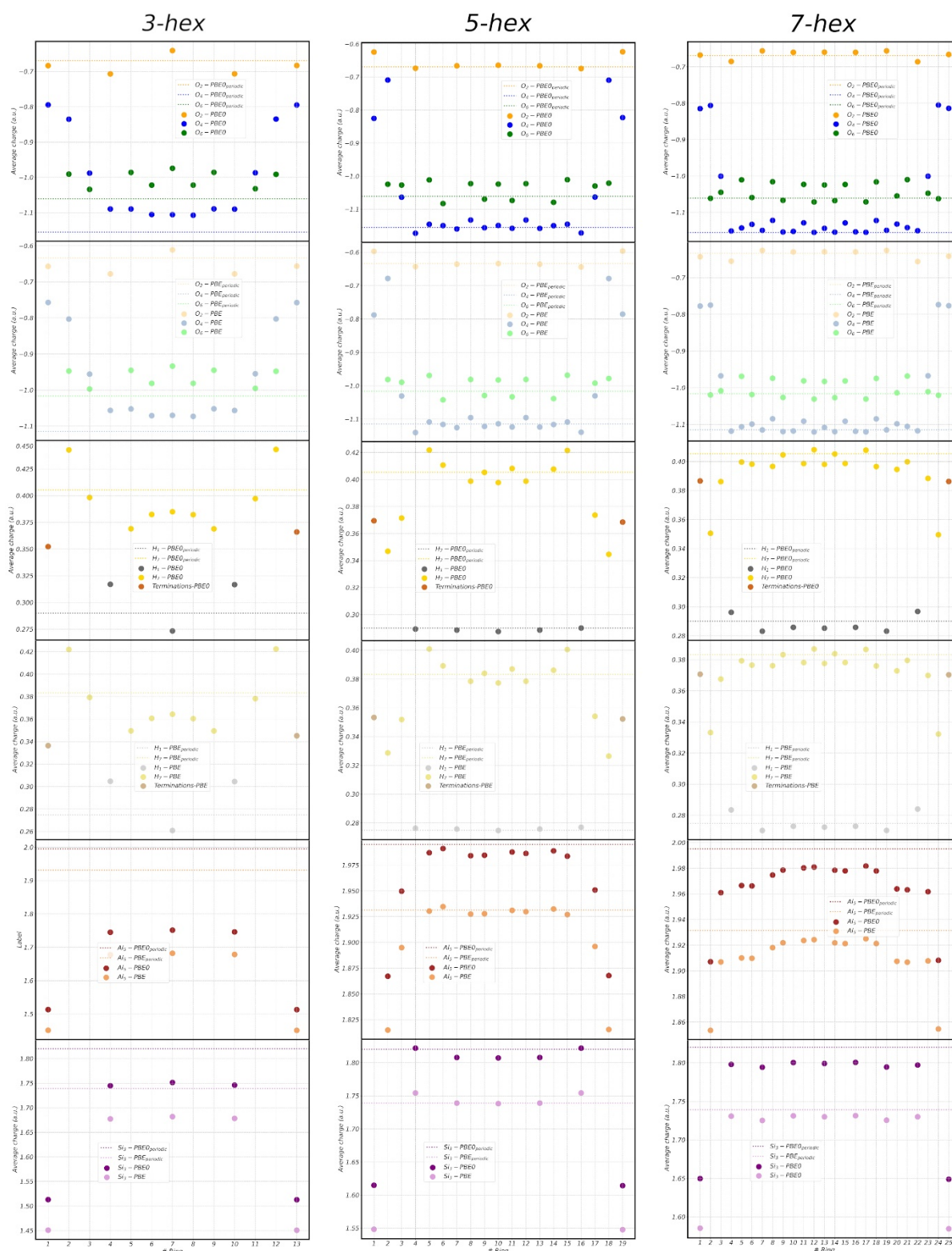


Figure 1. Ring-averaged, atom-resolved DDAPC charge (a.u.) for the hex-3, hex-5 and hex-7 models of the **OH-terminated** AlSi NT at PBE0-TC-LRC (shorthand notation: PBE0) and PBE level. For sake of clarity, the PBE and PBE0-TC-LRC results for the $O_{2,4,6}$ and $H_{1,7}$ atoms are displayed on different panels. The “Terminations” labeling is used to indicate the H-atoms belonging to the terminal OH groups saturating the terminal Si_3 -atoms (see Figure 1).

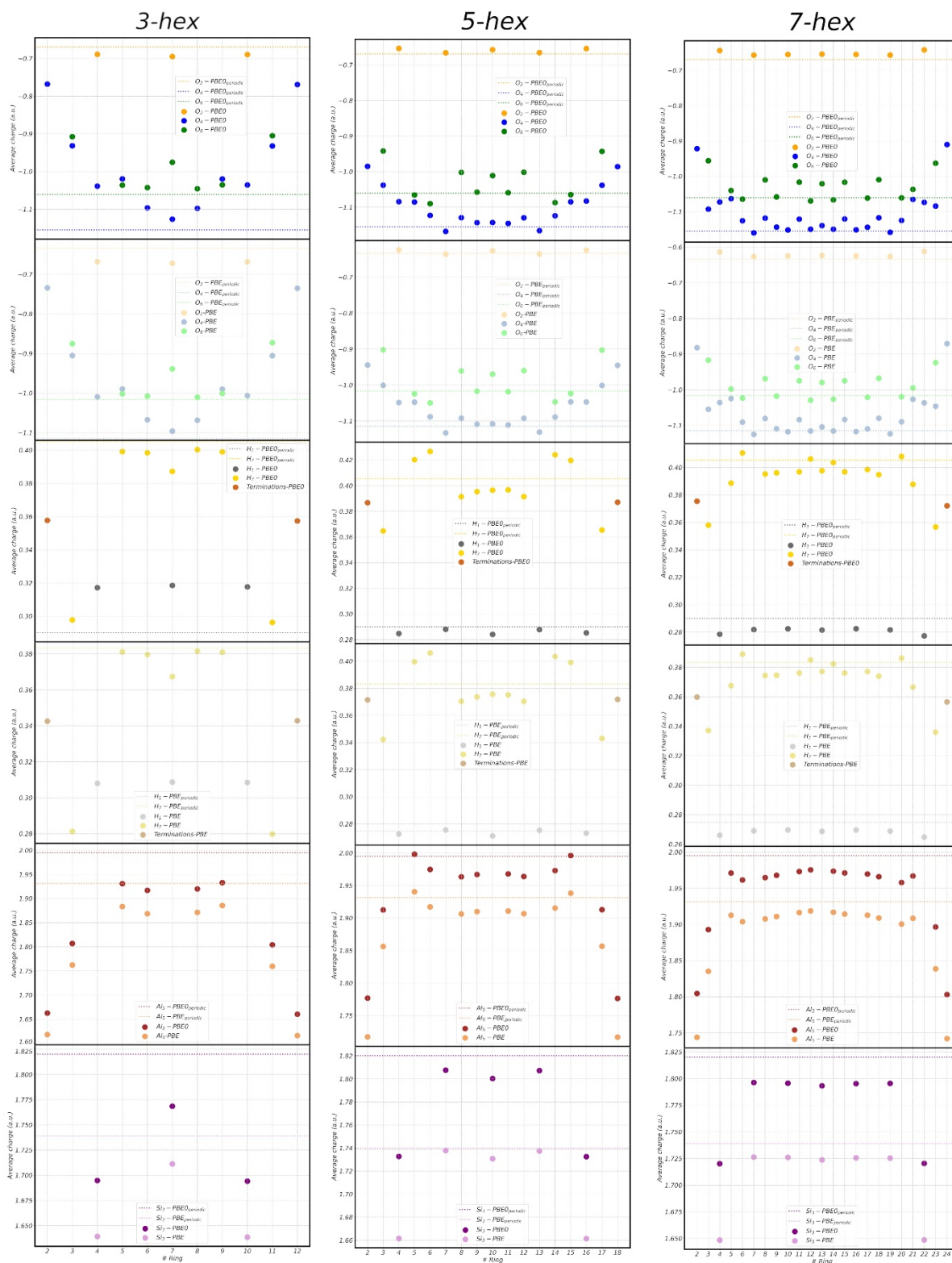


Figure 2. Ring-averaged, atom-resolved DDAPC charge (a.u.) for the hex-3, hex-5 and hex-7 models of the **H₂O-terminated** AlSi NT at PBE0-TC-LRC (shorthand notation: PBE0) and PBE level. For sake of clarity, the PBE and PBE0-TC-LRC results for the $O_{2,4,6}$ and $H_{1,7}$ atoms are displayed on different

panels. The “Terminations” labeling is used to indicate the H-atoms belonging to the terminal H₂O molecules saturating the terminal Al₅-atoms (see Figure 1).

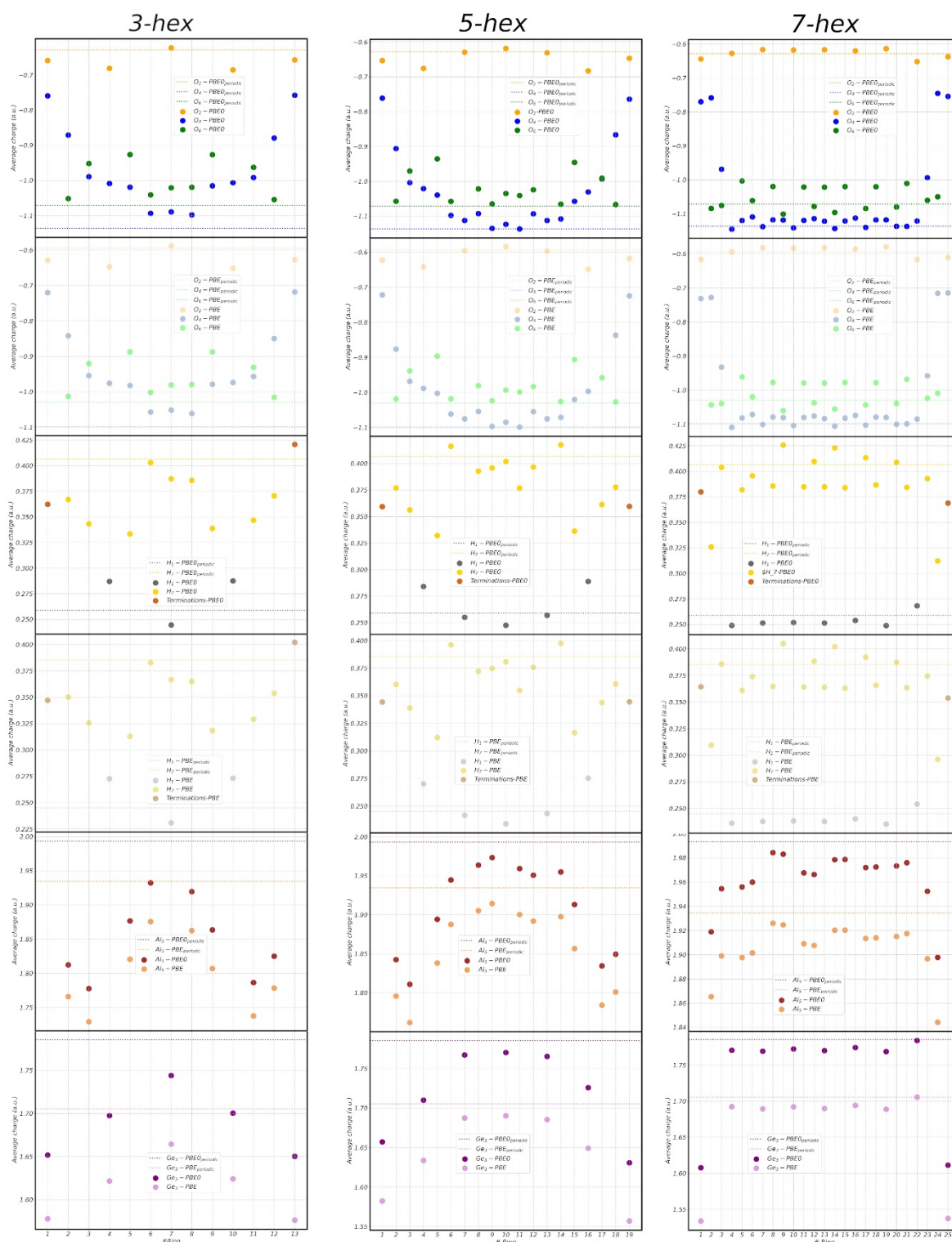


Figure 3. Ring-averaged, atom-resolved DDAPC charge (a.u.) for the hex-3, hex-5 and hex-7 models of the OH-terminated AlGe NT at PBE0-TC-LRC (shorthand notation: PBE0) and PBE level. For sake of clarity, the PBE and PBE0-TC-LRC results for the O_{2,4,6} and H_{1,7} atoms are displayed on different panels. The “Terminations” labeling is used to indicate the H-atoms belonging to the terminal OH groups saturating the terminal Ge₃-atoms (see Figure 1).

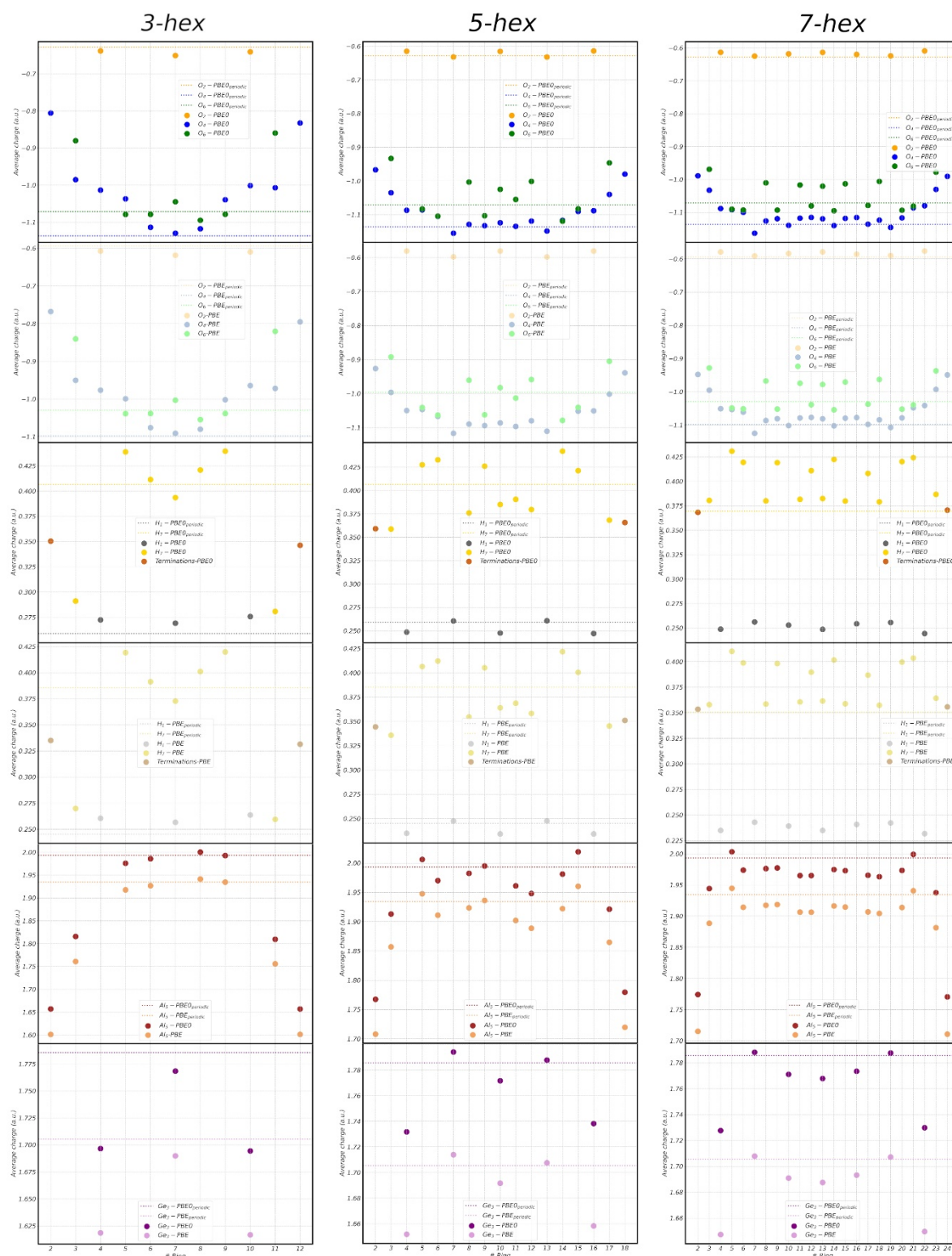


Figure 4. Ring-averaged, atom-resolved DDAPC charge (a.u.) for the hex-3, hex-5 and hex-7 models of the H_2O -terminated AlGe NT at PBE0-TC-LRC (shorthand notation: PBE0) and PBE level. For sake of clarity, the PBE and PBE0-TC-LRC results for the $\text{O}_{2,4,6}$ and $\text{H}_{1,7}$ atoms are displayed on different panels. The “Terminations” labeling is used to indicate the H-atoms belonging to the terminal H_2O molecules saturating the terminal Al_1 -atoms (see Figure 1).



