



- 1 Supplementary Material
- 2 Termination Effects in Aluminosilicate and
- 3 Aluminogermanate Imogolite Nanotubes: a Density
- 4 Functional Theory Study

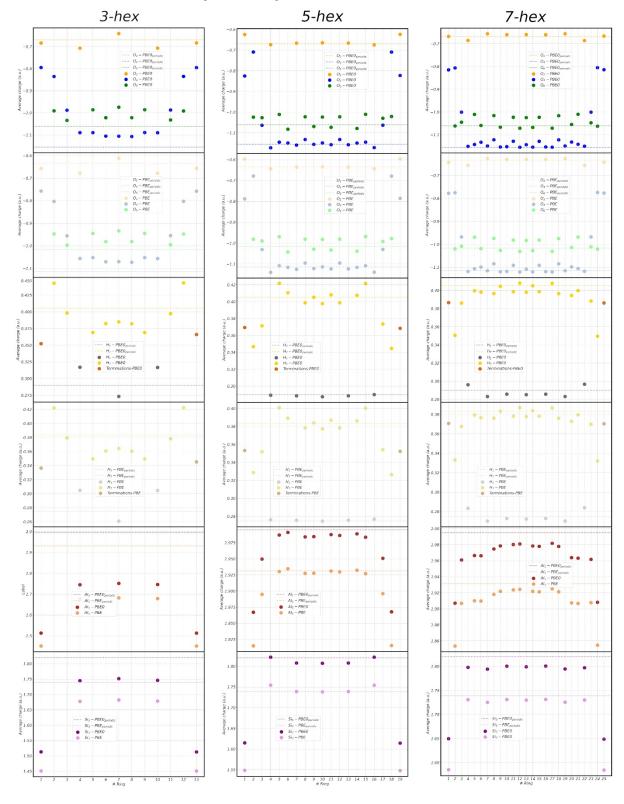


Figure 1. Ring-averaged, atom-resolved DDAPC charge (a.u.) for the hex-3, hex-5 and hex-7 models of the **OH-terminated AlSi NT** at PBE0-TC-LRC (shorthand notation: PBE0) and PBE level. For sake of clarity, the PBE and PBE0-TC-LRC results for the O_{2,4,6} and H_{1,7} atoms are displayed on different panels. The "Terminations" labeling is used to indicate the H-atoms belonging to the terminal OH groups saturating the terminal Si₃-atoms (see Figure 1).

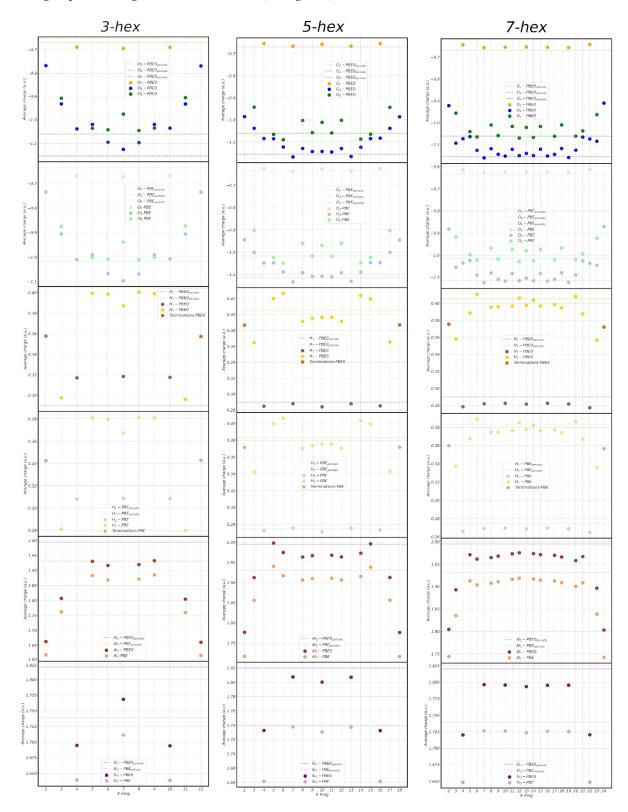
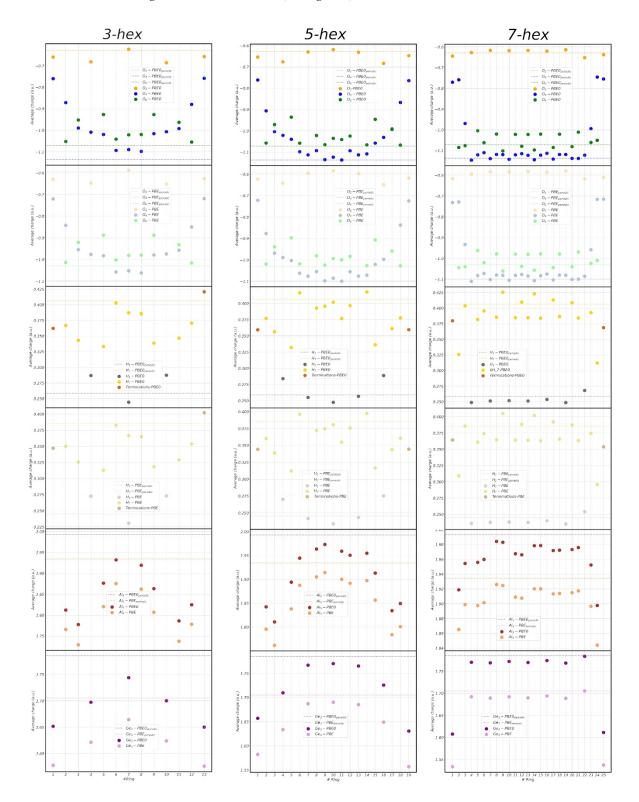




Figure 2. Ring-averaged, atom-resolved DDAPC charge (a.u.) for the hex-3, hex-5 and hex-7 models of the H2O-terminated AlSi NT at PBE0-TC-LRC (shorthand notation: PBE0) and PBE level. For sake of clarity, the PBE and PBE0-TC-LRC results for the O_{2,4,6} and H_{1,7} atoms are displayed on different



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).



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18Figure 3. Ring-averaged, atom-resolved DDAPC charge (a.u.) for the hex-3, hex-5 and hex-7 models19of the OH-terminated AlGe NT at PBE0-TC-LRC (shorthand notation: PBE0) and PBE level. For sake20of clarity, the PBE and PBE0-TC-LRC results for the O2,4,6 and H1,7 atoms are displayed on different21panels. The "Terminations" labeling is used to indicate the H-atoms belonging to the terminal OH22groups saturating the terminal Ge3-atoms (see Figure 1).

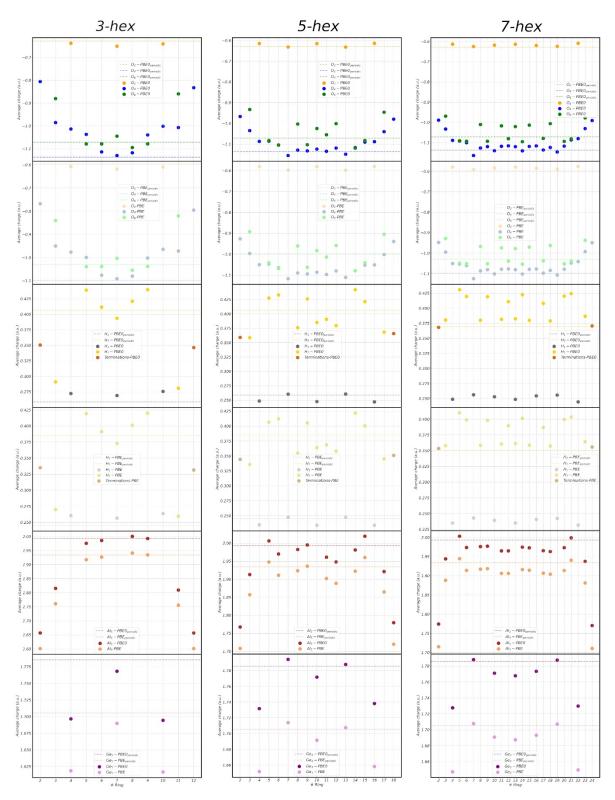


Figure 4. Ring-averaged, atom-resolved DDAPC charge (a.u.) for the hex-3, hex-5 and hex-7 models of the H₂O-terminated AlGe NT at PBE0-TC-LRC (shorthand notation: PBE0) and PBE level. For sake of clarity, the PBE and PBE0-TC-LRC results for the O_{2,4,6} and H_{1,7} atoms are displayed on different panels. The "Terminations" labeling is used to indicate the H-atoms belonging to the terminal H₂O molecules saturating the terminal Al₅-atoms (see Figure 1).



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