Boron Nitride Nanotube Nucleation during Ni-catalysed Boron Oxide Chemical Vapor Deposition

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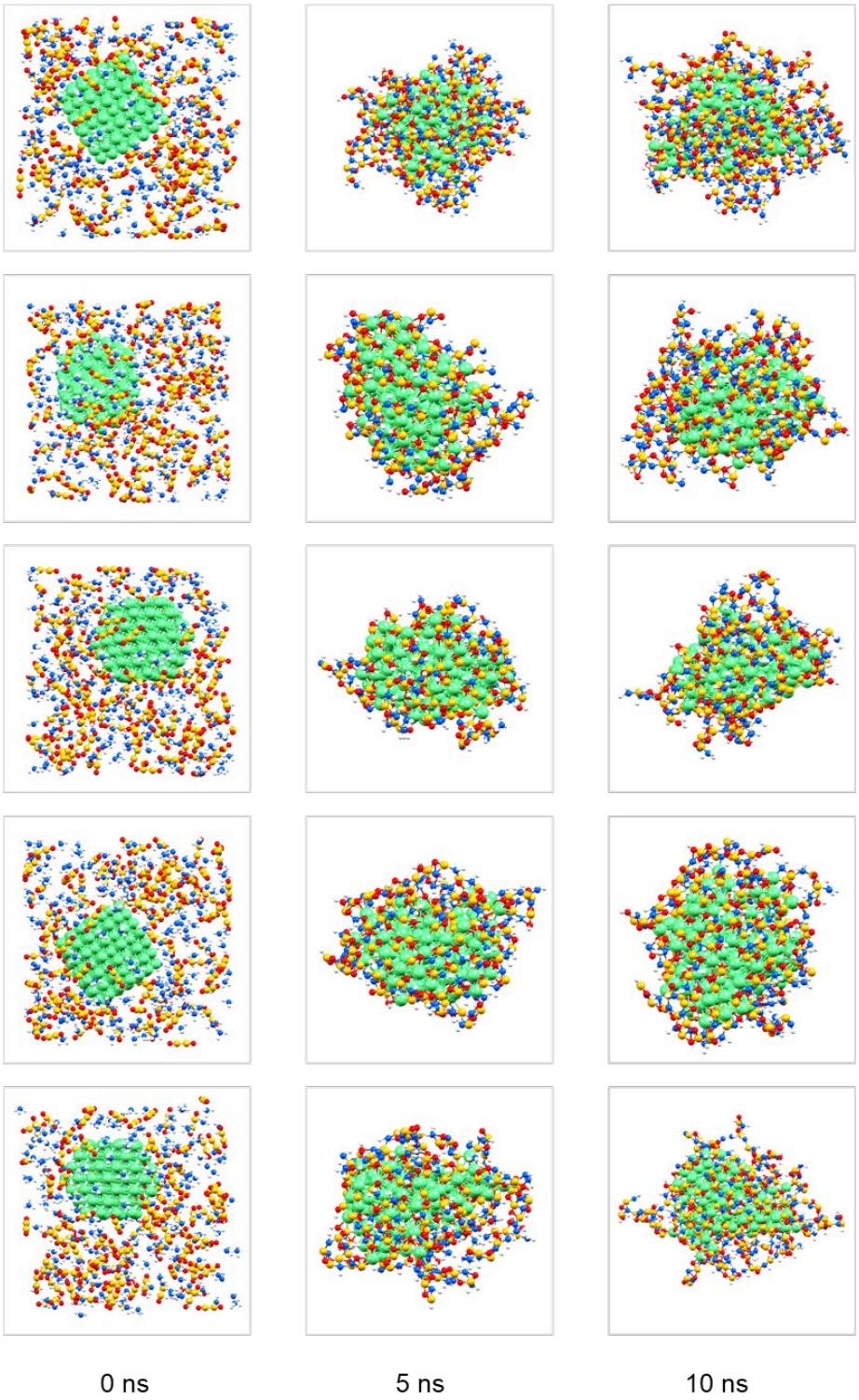

Figure S1. Simulation boxes at 0 ns, 5 ns and 10 ns. For 5 ns and 10 ns, the image is zoomed in on the Ni catalyst particle. Green, blue, yellow red and white spheres represent Ni, N, B, O and H atoms, respectively.

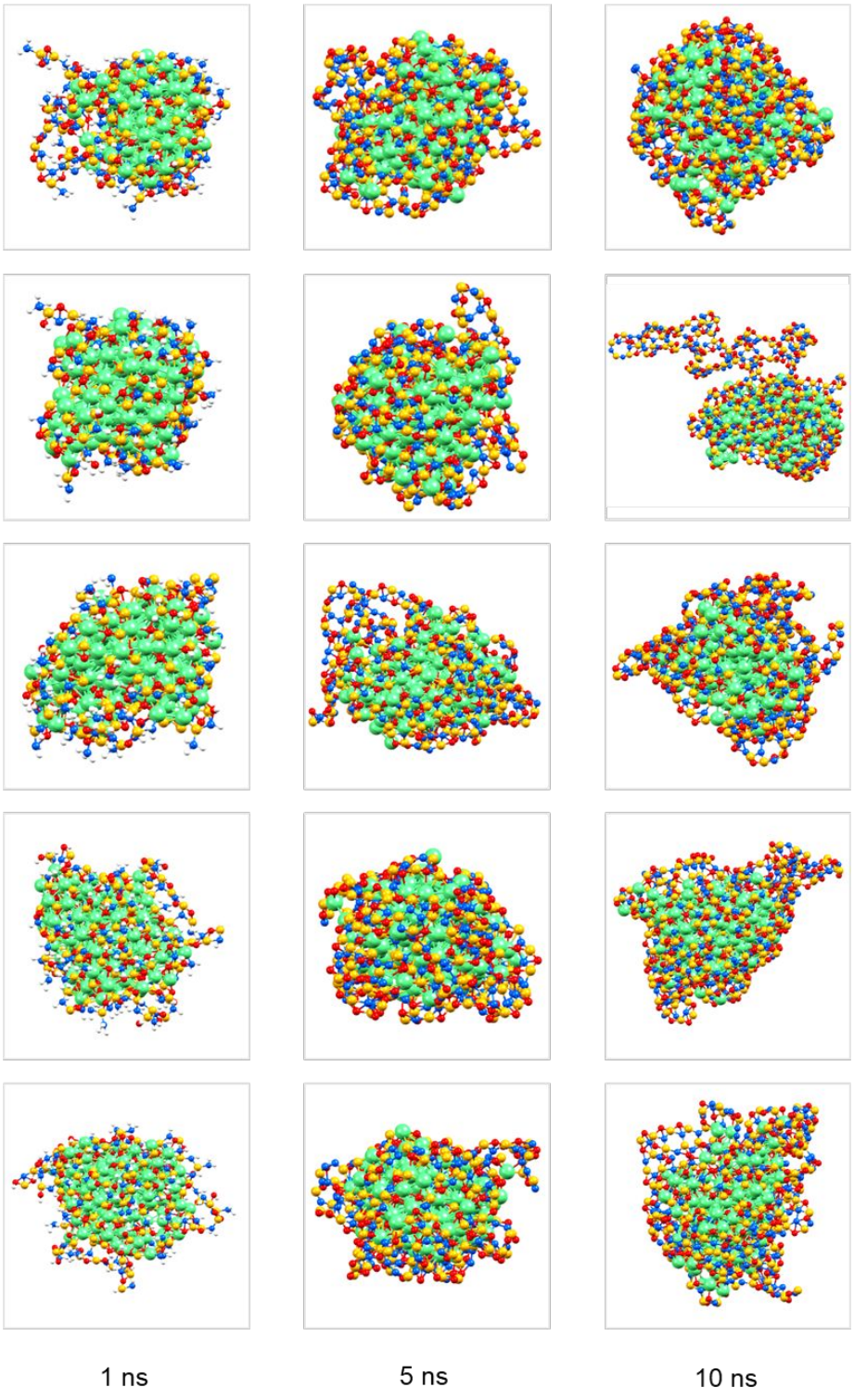

Figure S2. Ni_{147} catalyst surface at 0 ns, 5 ns and 10 ns following the periodic removal of H_2. Atom colours as per Figure S1.

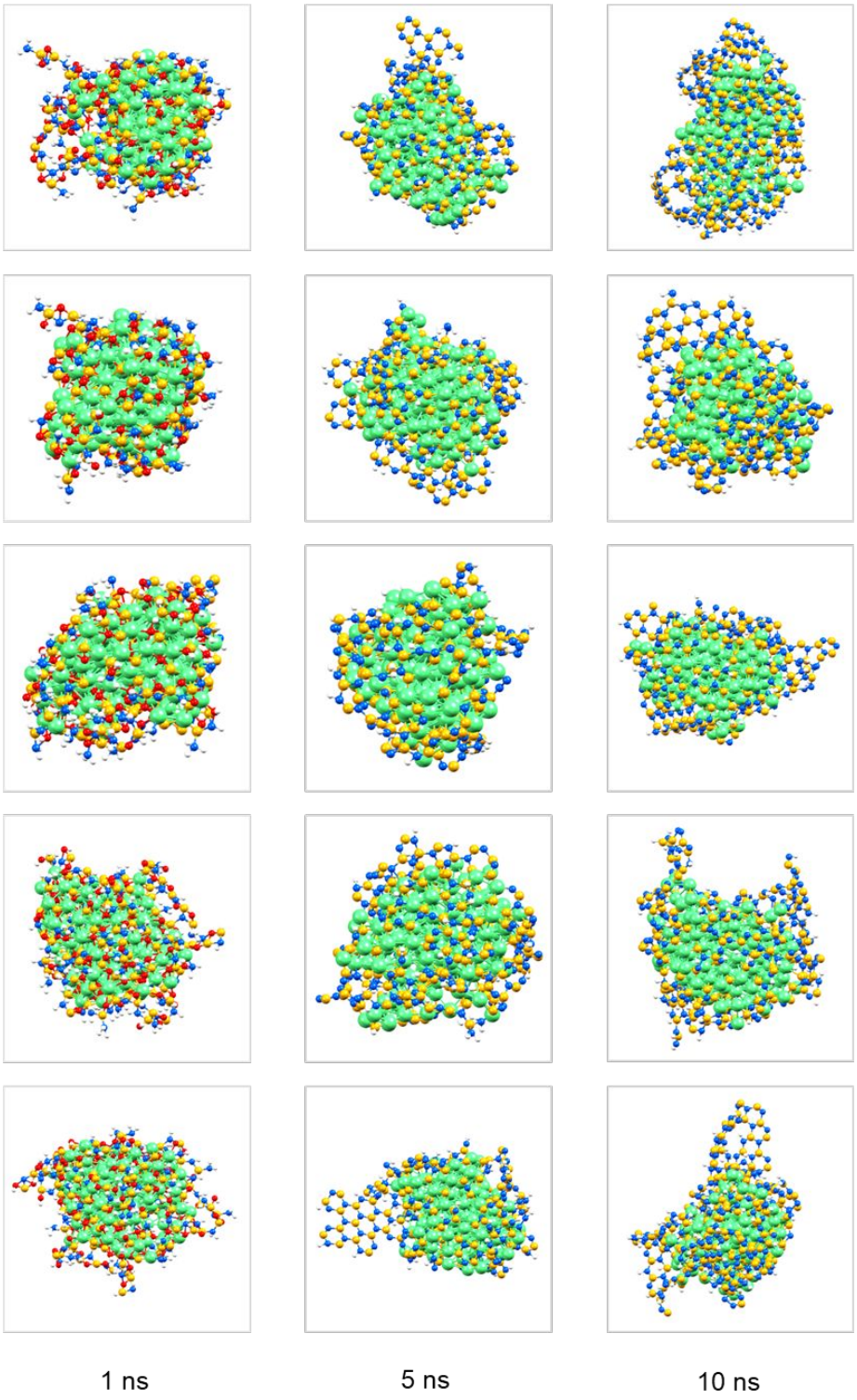

Figure S3. Ni_{147} catalyst surface at 0 ns, 5 ns and 10 ns following the periodic removal of H_2O. Atom colours as per Figure S1.

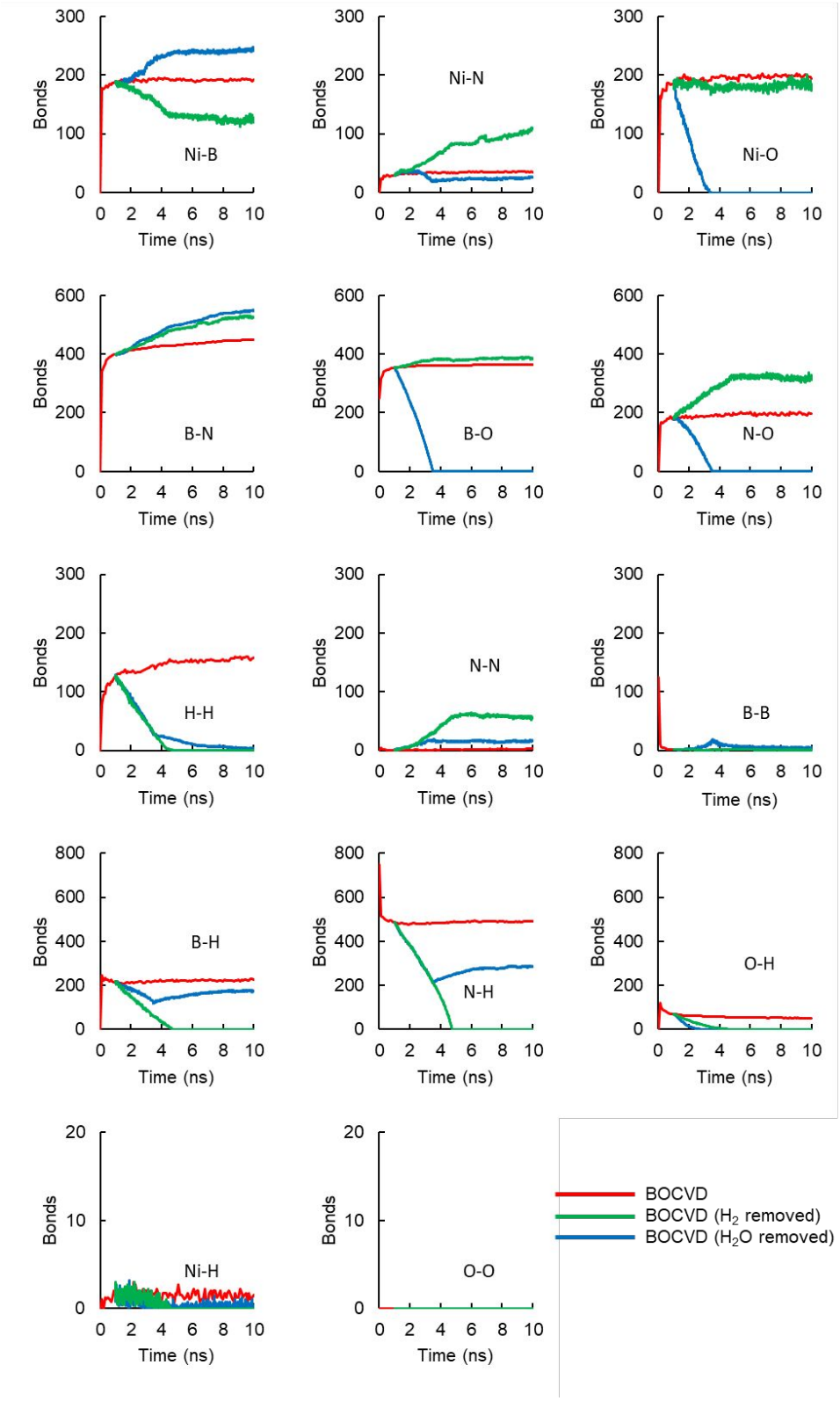

Figure S4. Populations of all bonds present over 10 ns across all BOCVD simulations.

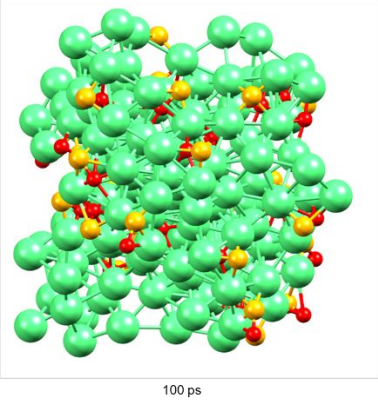

Figure S5. Free BO monomers (24) adsorbed to the Ni_{147} catalyst after 100 ps of simulation. Atom colours as per Figure S1.

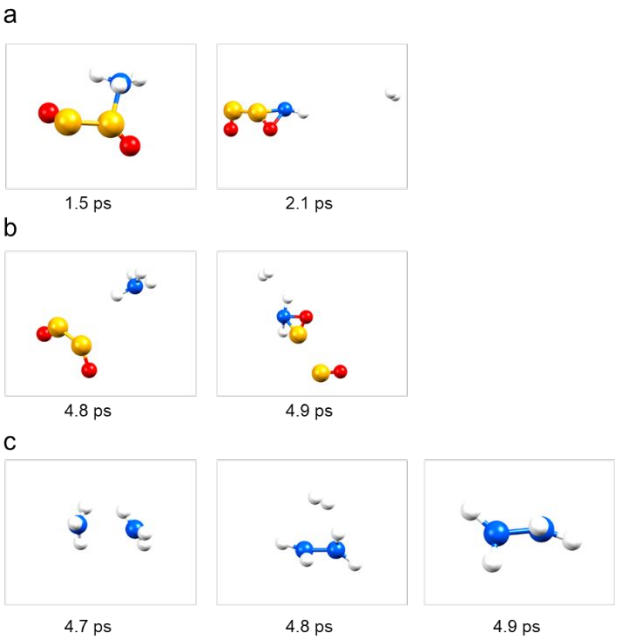

Figure S6. (a) H_2 release from B_2O_2 and NH_3 reaction product in gas-phase. (b) H_2 release from B_2O_2 and NH_4 reaction product in gas-phase. (c) H_2 release from N_2H_6 dimer in gas-phase. Atom colours per Figure S1.

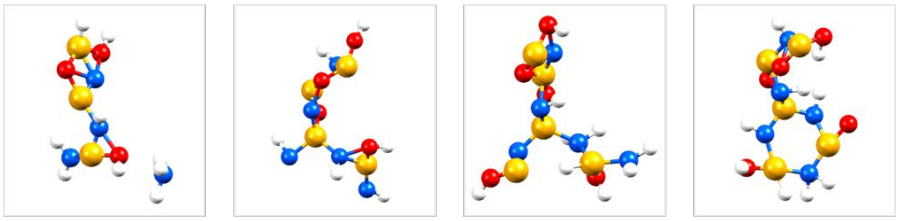

Figure S7. Growth of BN chain via addition of NH_2 and BOH groups and chain oligomerisation leading to closure of hexagonal BN ring in the gas-phase. Atom colours per Figure S1.

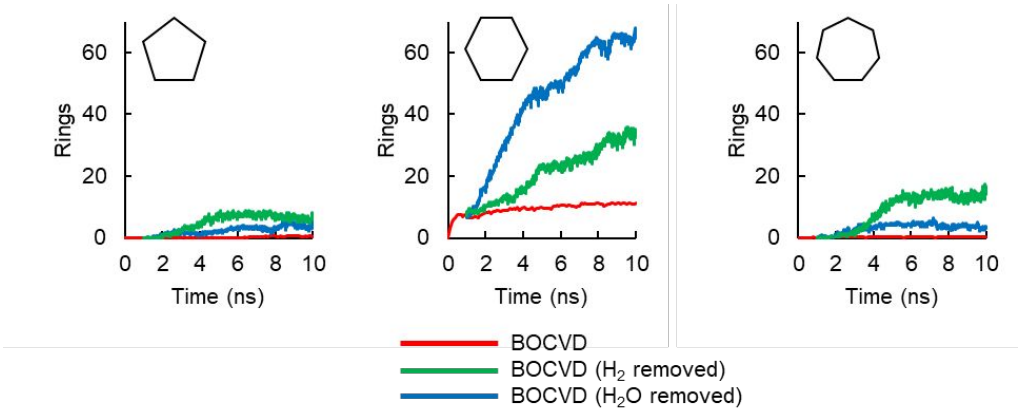

Figure S8. Populations of pentagons, hexagons and heptagons over 10 ns across all BOCVD simulations.

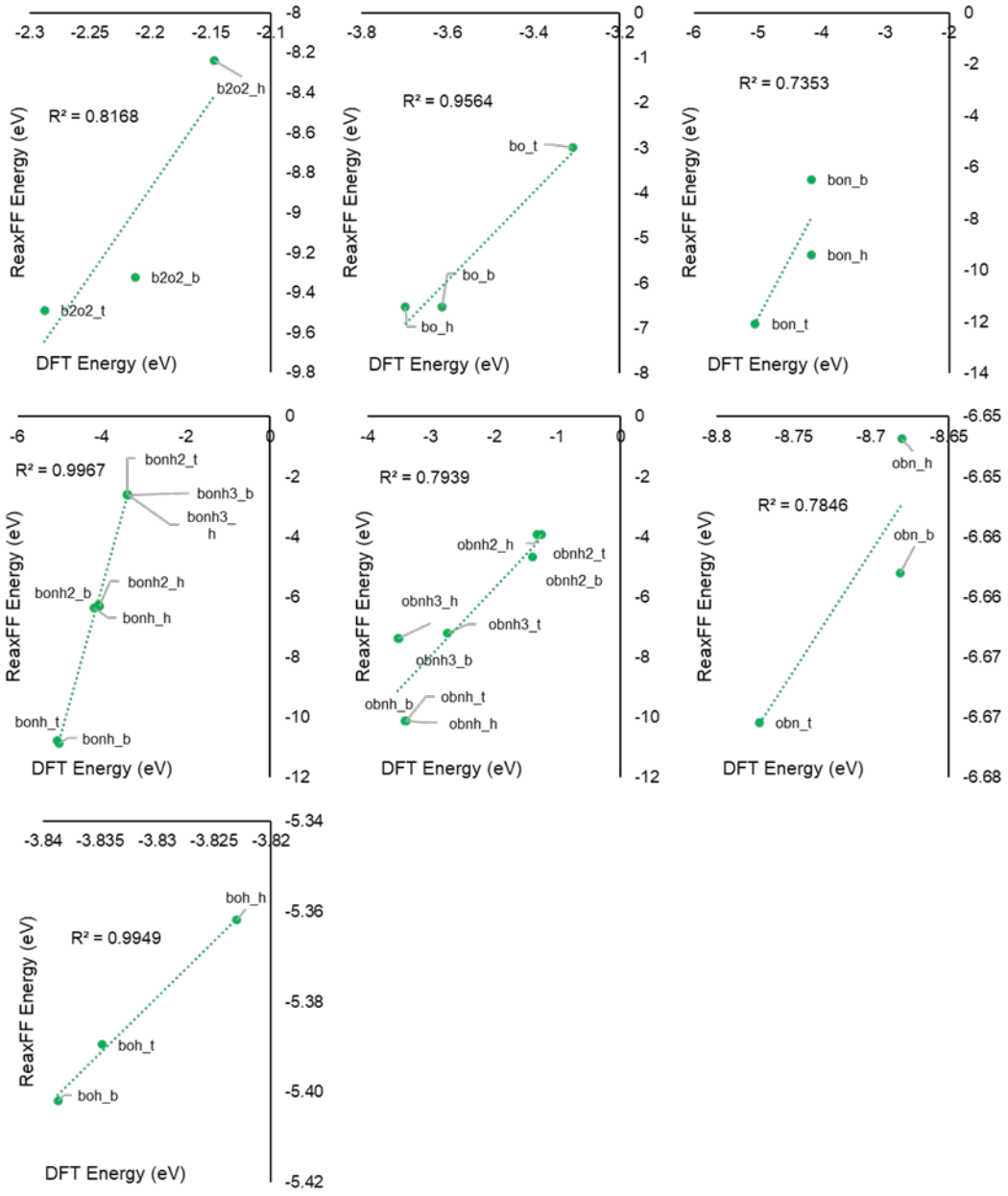

Figure S9. Comparison of ReaxFF (vertical axis) and PBE (horizontal axis) adsorption energies (eV) of pertinent $B_xO_xN_yH_z$ species observed during BOCVD and BNNT nucleation. All calculations employ a 4x4x5 Ni(111) slab model. In data labels, the fragment name is organised to detail the structure (e.g. BON indicates the O is bonded to the N where OBN indicates the B is bonded to N) and b, h and t standing for bridge site, hollow site and top site absorption of the fragment in the geometry prior to optimisation. Adsorption energy is defined as $E_{ads}=E_{Ni+BxOxNyHz} - (E_{Ni} + E_{BxOxNyHz})$.

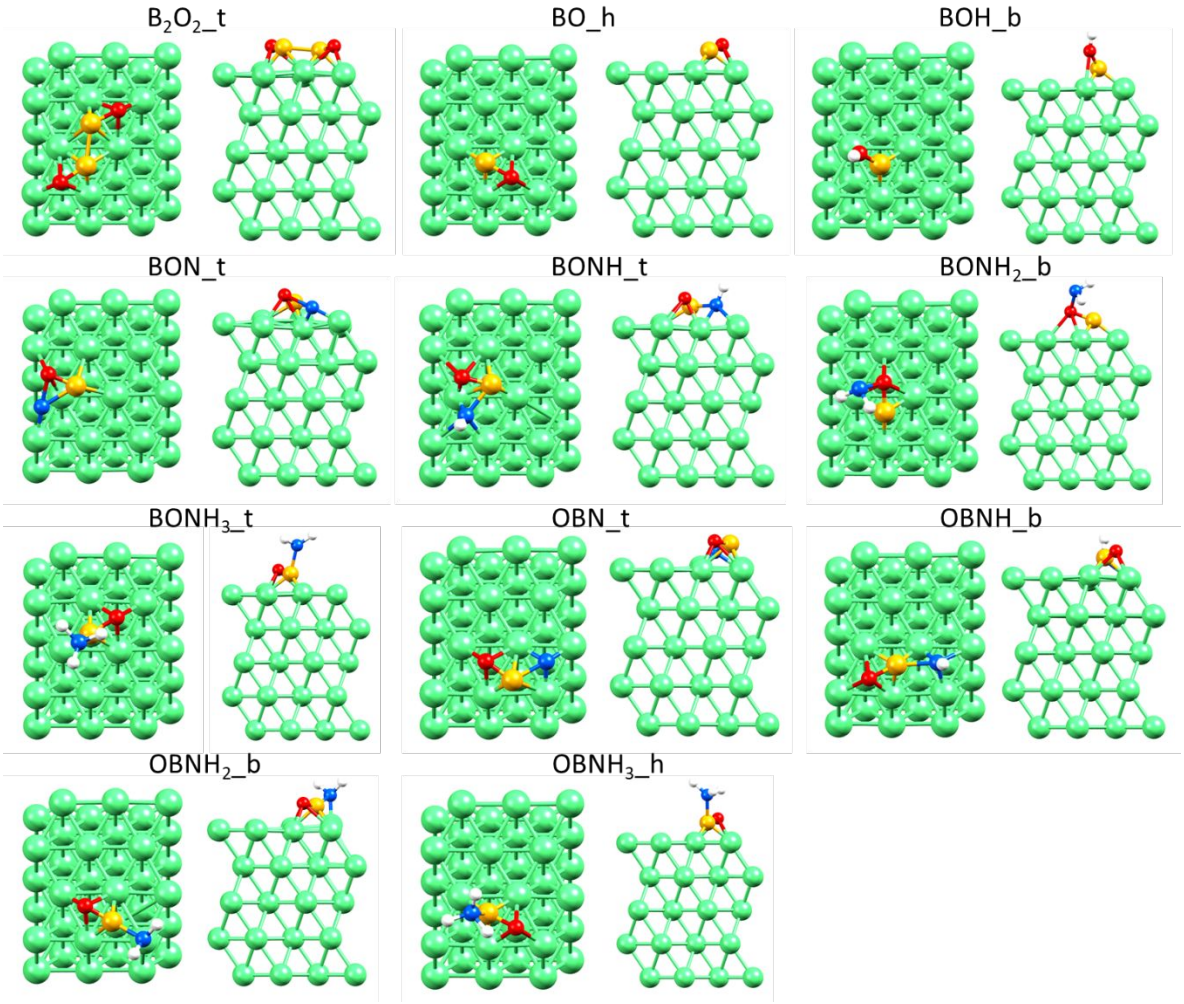

Figure S10. Lowest energy geometry for each $B_xO_xN_yH_z$ fragment adsorbed on Ni. In data labels, the fragment name is organised to detail the structure (e.g. BON indicates the O is bonded to the N where OBN indicates the B is bonded to N) and b, h and t standing for bridge site, hollow site and top site absorption of the fragment in the geometry prior to optimisation. Atom colours per Figure S1.