## Supporting information for "CNH monolayer: a direct gap 2D semiconductor with anisotropic electronic and optical properties"

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Fig. S1 The final structure after MD simulation of  $\alpha$ -CNH at a certain temperature for 10 *ps* of (a) 700K, (b) 800K, (c) 1000K, respectively.



Fig. S2 The different configurations and band structures of  $\alpha$ -CNH bilayer. (a) structure A<sub>2</sub>B<sub>1</sub>, E<sub>g</sub>=1.67 eV,  $\Delta$ E=0.00 meV; (b) structure A<sub>1</sub>B<sub>1</sub>, E<sub>g</sub>=1.67 eV,  $\Delta$ E=25.15 meV; (c) structure A<sub>2</sub>B<sub>2</sub>, E<sub>g</sub>=1.64 eV,  $\Delta$ E=67.93 meV; (d) structure A<sub>1</sub>B<sub>2</sub>, E<sub>g</sub>=1.65 eV,  $\Delta$ E=74.81 meV. respectively. 'A' represent the right view and 'B' represent the left view, '1' represent the second layer is just on the top of first layer in current view and '2' represent interlaced layers in current view. E<sub>g</sub> is the value of band gap;  $\Delta$ E=E<sub>total</sub>-E<sub>ref</sub>, E<sub>total</sub> is the total energy and E<sub>ref</sub> is energy of reference configuration (A<sub>1</sub>B<sub>1</sub>).



Fig. S3 The relationship between the total energy and the distance of two layers of  $\alpha$ -CNH.



Fig. S4 (a) The structures and band structures of 3-layers  $\alpha$ -CNH, E<sub>g</sub>=1.65 eV; (b) the structures and band structures of 4-layers  $\alpha$ -CNH, E<sub>g</sub>=1.63 eV, E<sub>g</sub> is the value of band gap.