

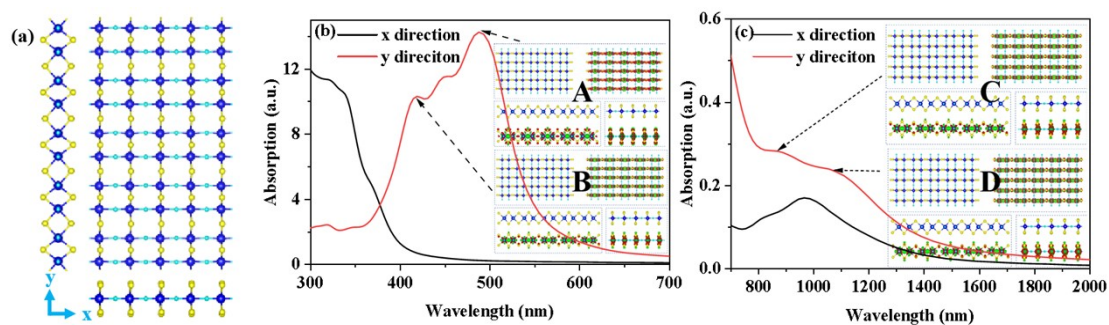
Supporting information

Indirect and direct electronic transitions and electron transport properties of van der Waals NbOCl₂

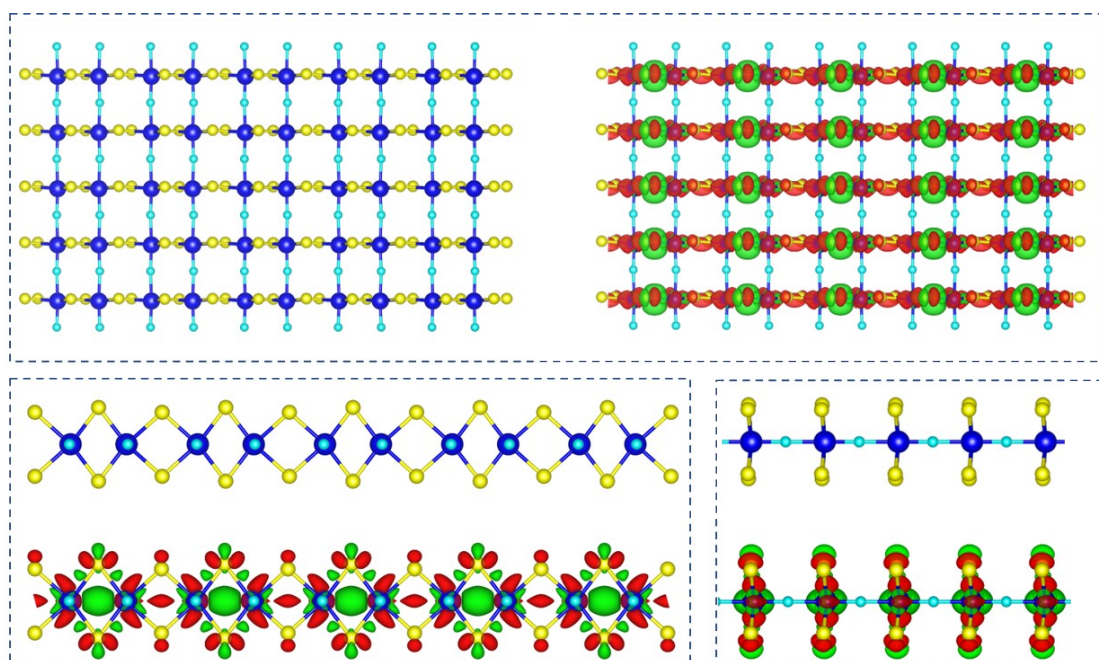
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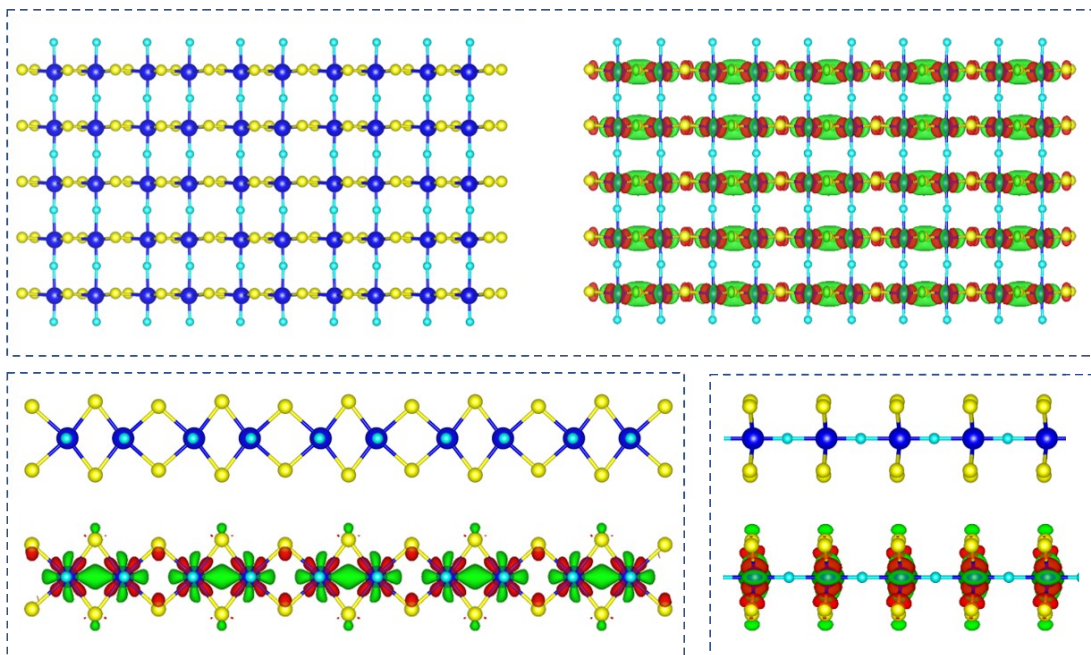
* Corresponding Author. Email: mengtaosun@ustb.edu.cn (M. Sun).



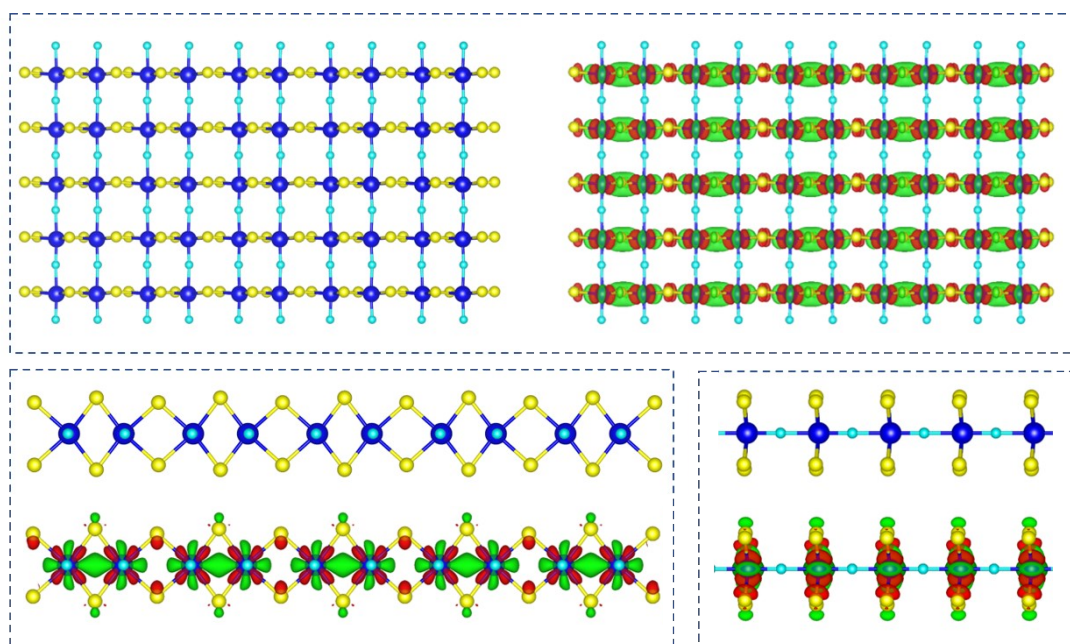
A



B



C



D

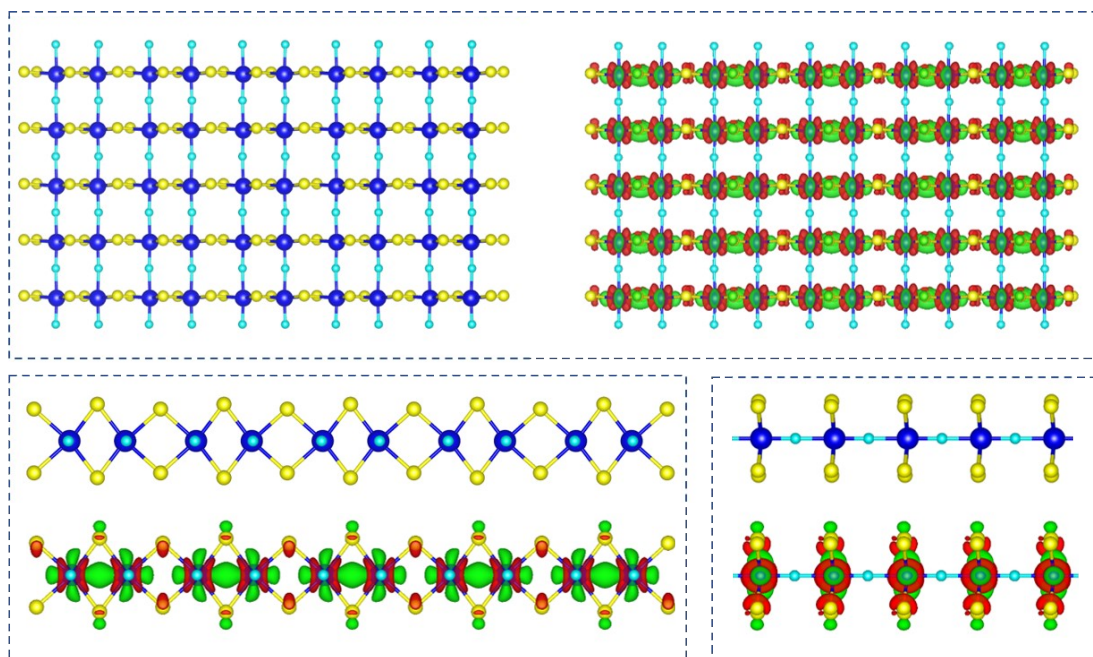


Figure S1. (a) Three views of the monolayer NbOCl₂. The blue atom is the metal Nb, the yellow atom is Cl, and the cyan atom is O. (b)(c) Absorption spectrum in the ultraviolet-visible region and the infrared region of the monolayer NbOCl₂, and the embedded graphs A, B, C and D (the charge transfer of absorption peaks in direction y are also shown respectively).

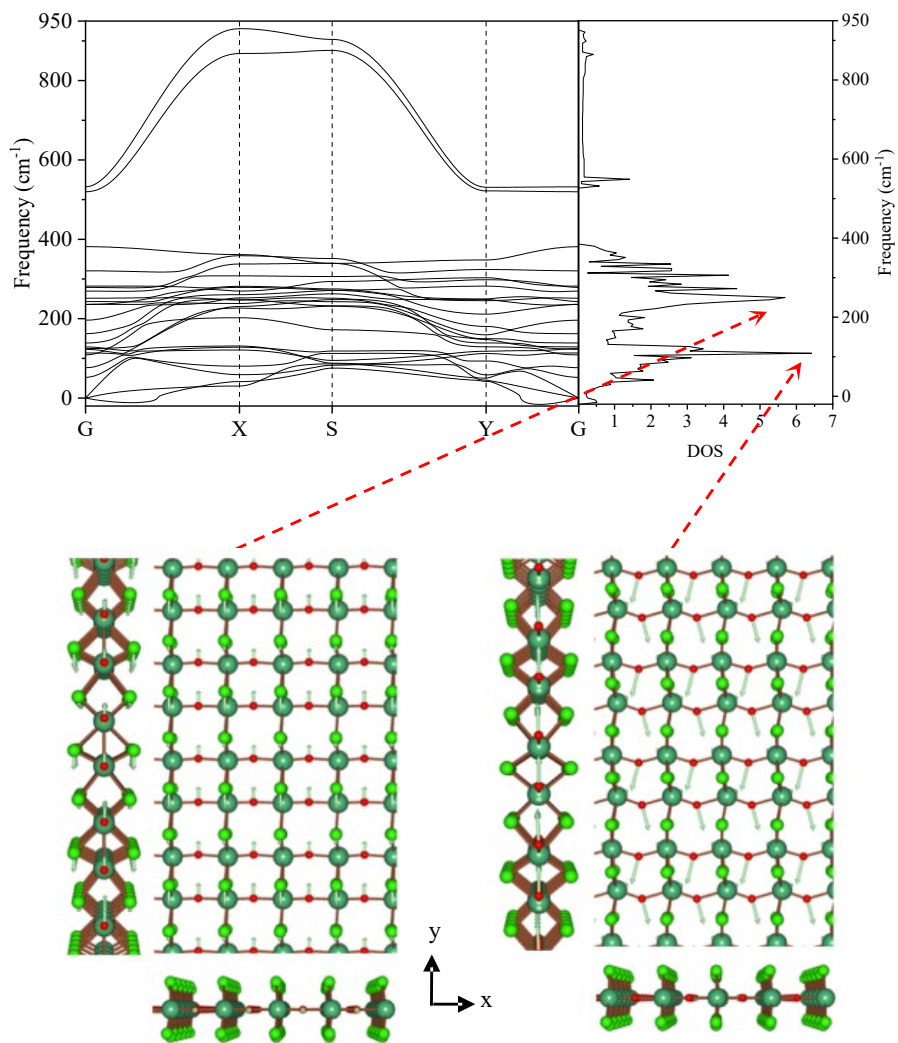
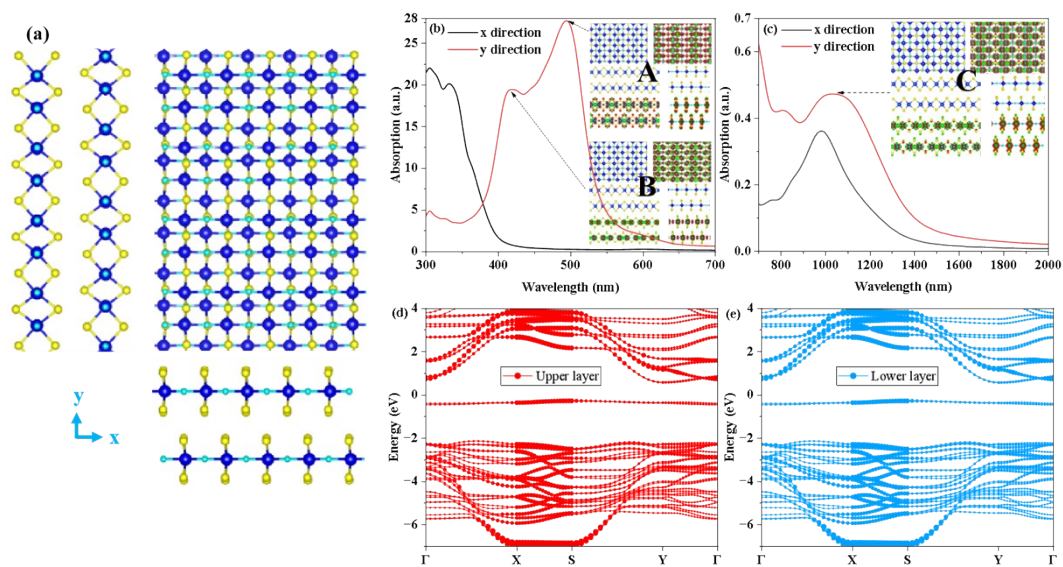
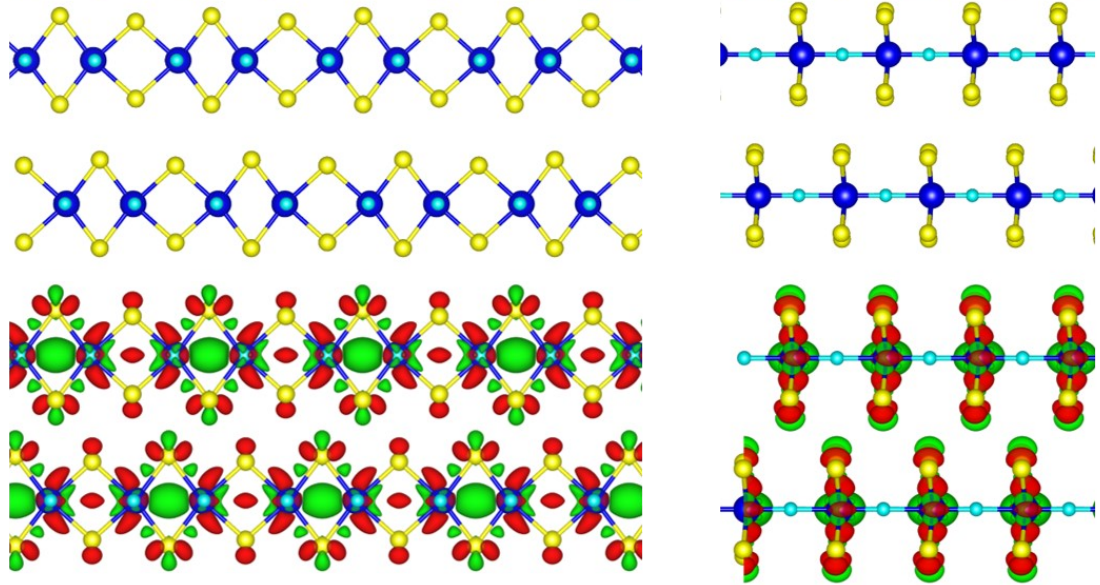
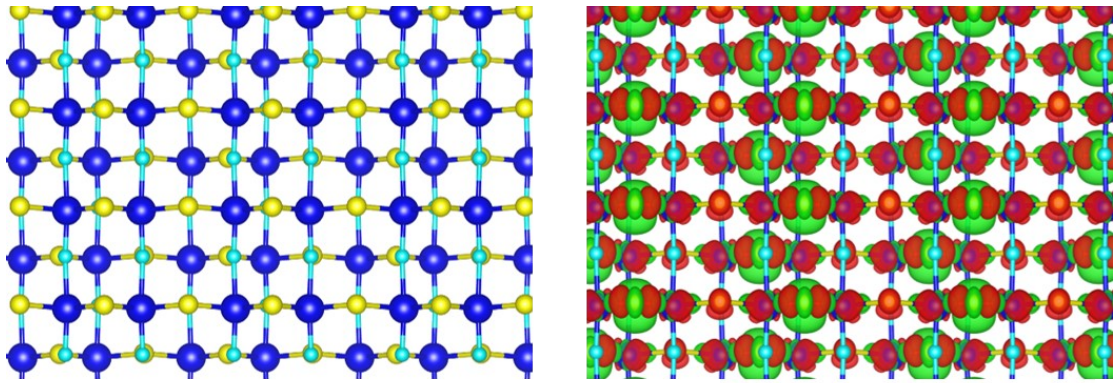


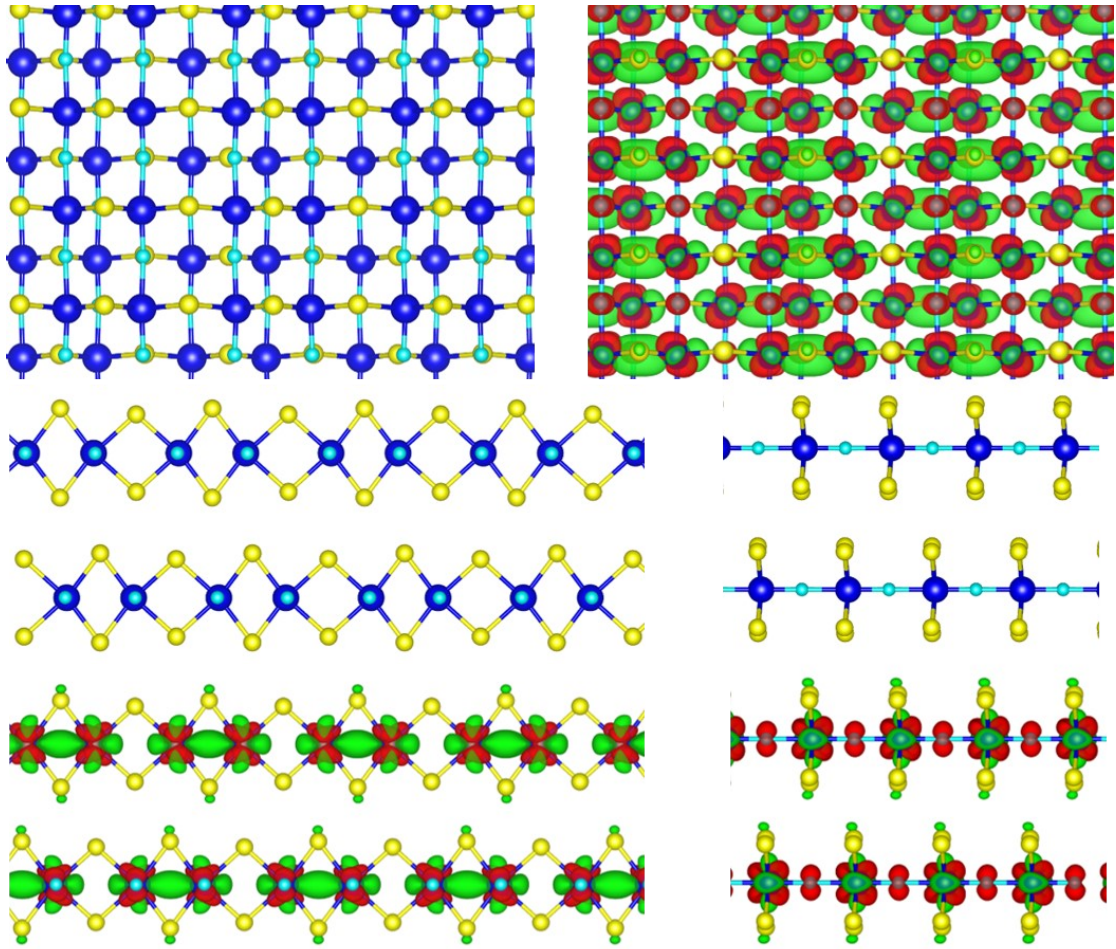
Figure S2. Vibration modes corresponding to the peaks of phonon DOS of monolayer NbOCl₂. the dark green atom is the metal Nb, the light green atom is Cl, and the red atom is O.



A



B



C

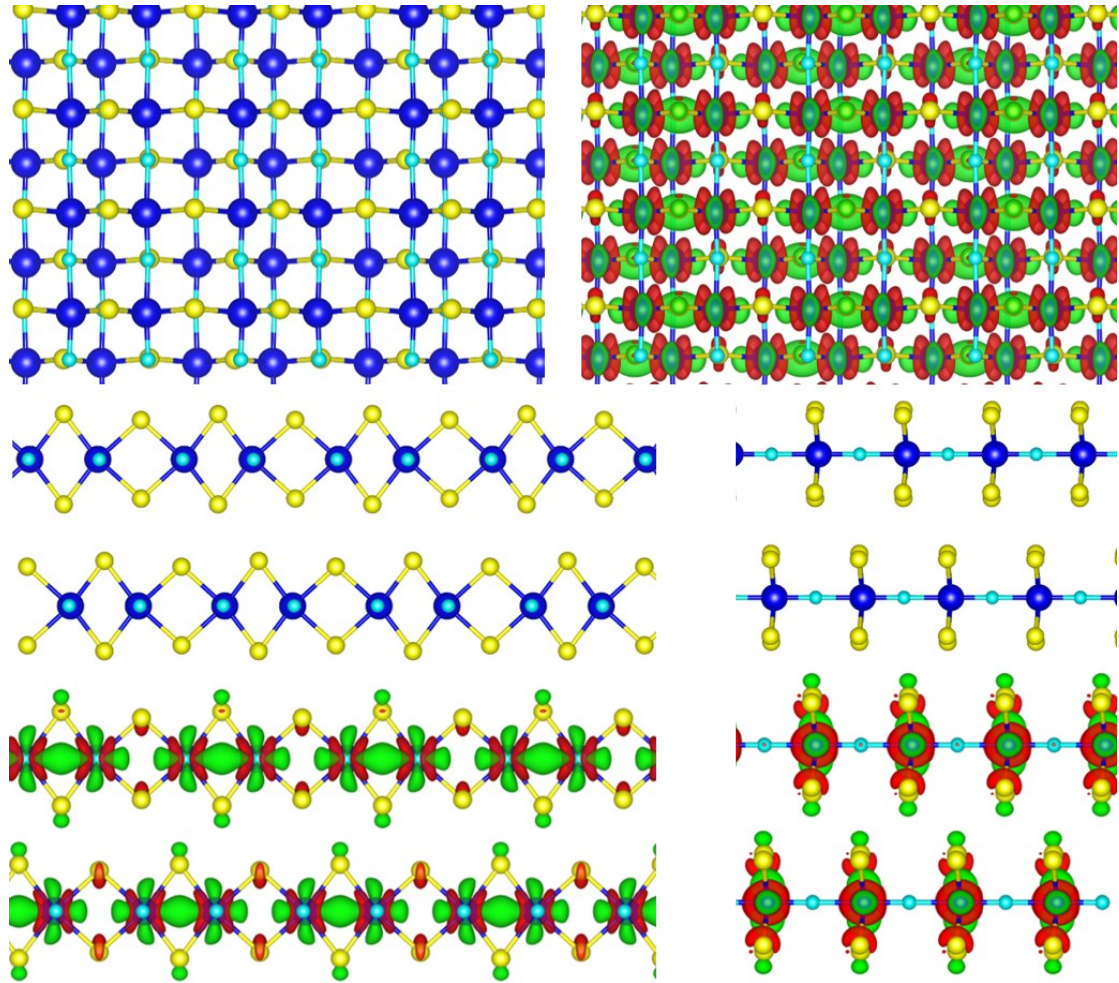


Figure S3. (a) Three views of the bilayer NbOCl₂. (b)(c) Absorption spectrum in the ultraviolet-visible region and the infrared region of the bilayer NbOCl₂, and the embedded graphs A, B, and C (the charge transfer of absorption peaks in direction y are also shown respectively). (d)(e) Energy band of the upper NbOCl₂ and the lower NbOCl₂.

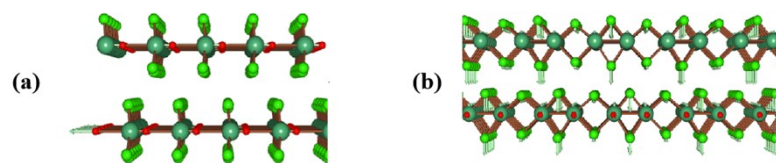


Figure S4. Vibration modes of the strongest peaks in (a) IR and (b) Raman spectrum of the bilayer NbOCl₂.

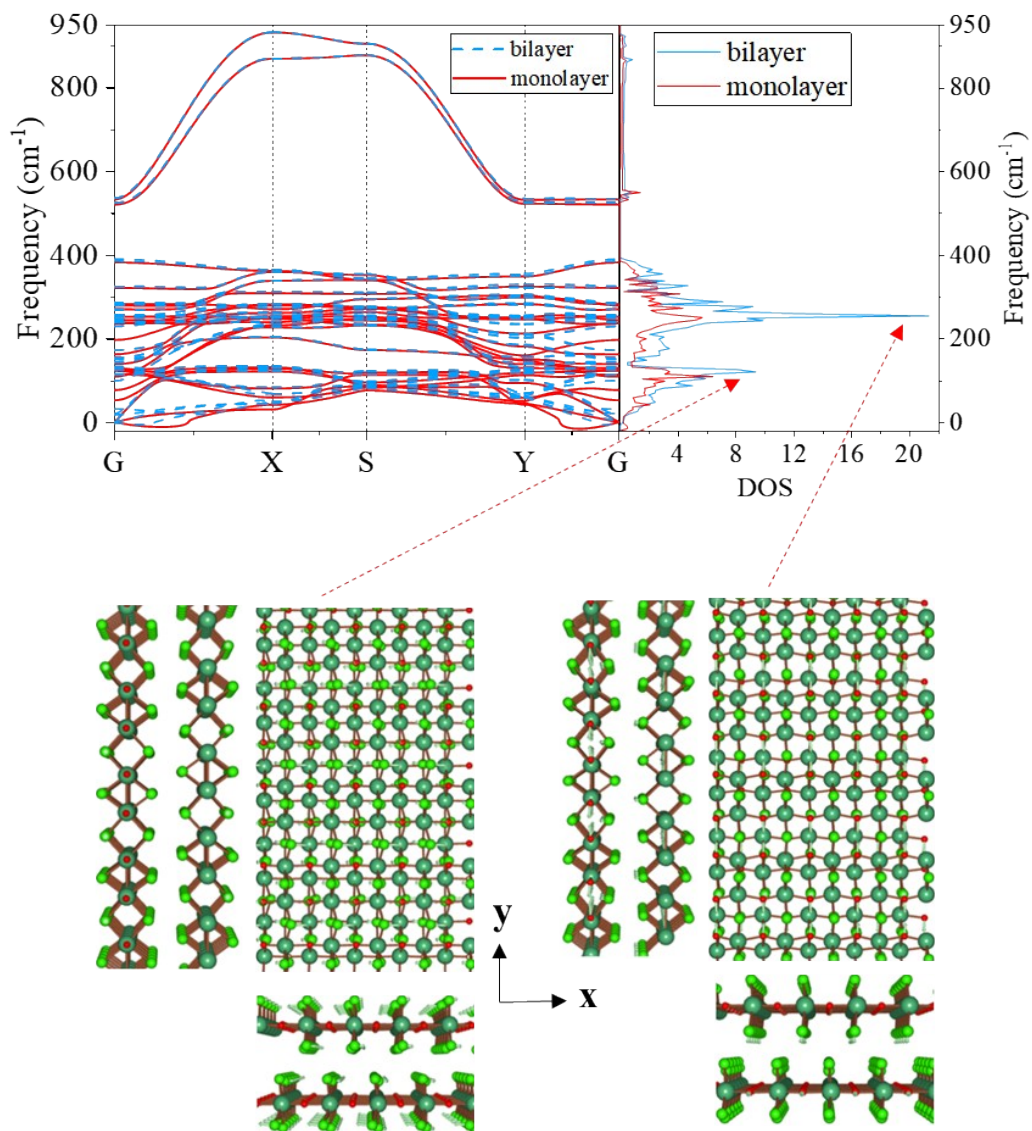


Figure S5. Vibration modes corresponding to the peaks of phonon DOS of bilayer NbOCl₂.