Supplementary Information for

Two-Dimensional Hexagonal CrN with Promising Magnetic and Optical Properties: A Theoretical Prediction

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In search of a 2D CrN atomic structure, at the initial stage we determine an equilibrium geometry of the CrN unit cell with the space group symmetry Fm-3m by using DFT+U method with 12 × 12 × 12 *k*-points mesh. The cell contained four Cr and four N atoms was chosen. The geometry optimization of bulk CrN demonstrates that the *a* translation vector equal to 4.227 Å which is in a good agreement with experimental data (a = 4.148 Å).[1]

The equilibrium geometries of $MoSe_2$ and MoS_2 unit cells of monolayers were calculated to study interaction of *h*-CrN with them. The k-point samplings of the first Brillouin zone (1BZ) have been chosen as 21 × 21 × 1 according to the Monkhorst–Pack scheme. The *a* translation vectors (3.294 Å and 3.165 Å for $MoSe_2$ and MoS_2 respectively) are in a good agreement with experimental data (a_{MoSe2} = 3.288 and a_{MoS2} = 3.15 Å)[2,3] and theoretical predicted ones (3.29 Å and 3.13 Å respectively).[4,5]

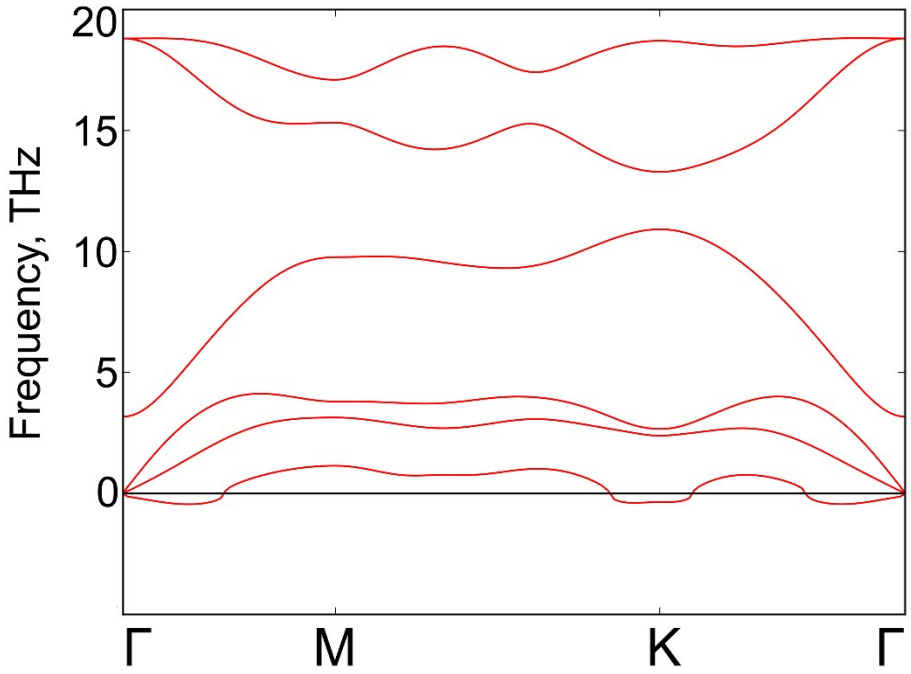

Figure S1. Phonon dispersion plot of the *h*-CrN sheet calculated using DFPT theory.

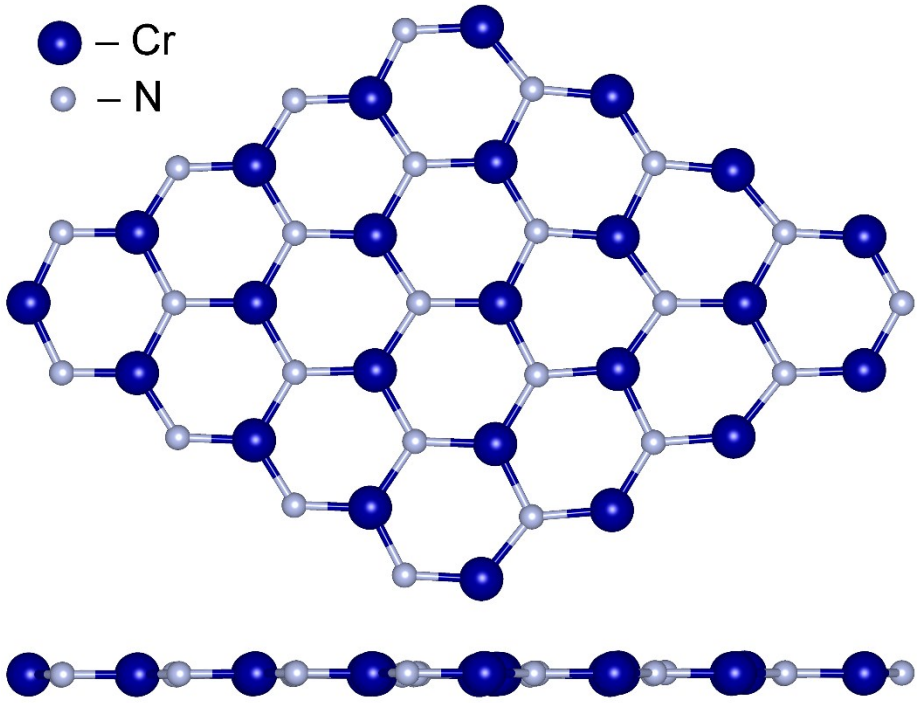

Figure S2. Equilibrium structure of the *h*-CrN nanocluster.

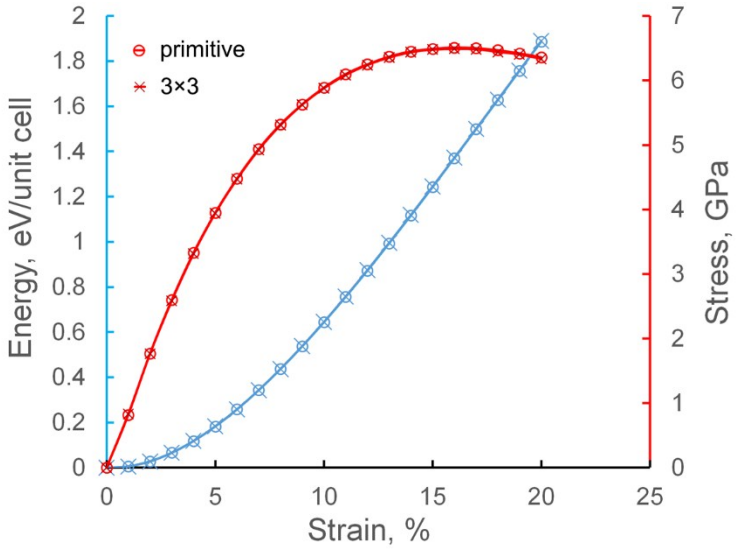

Figure S3. Equi-biaxial strain vs. energy (blue) and vs stress (red) plot for *h*-CrN. The strain energies as well as stress of both primitive and 3×3 cells are same.

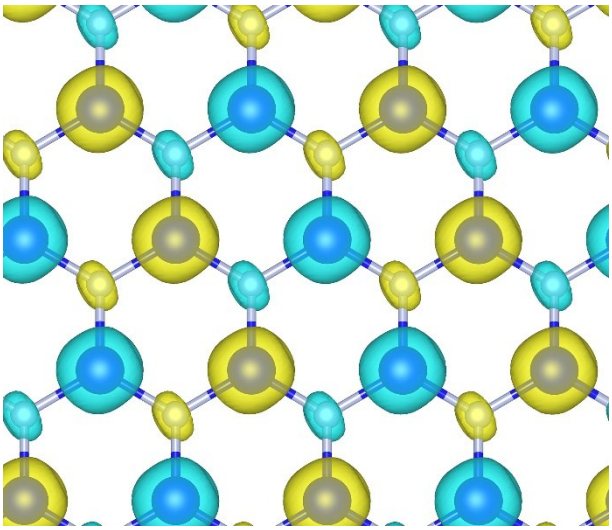

Figure S4. Isosurface (0.02 e/Å^3) of spatial spin density distribution of *h*-CrN AFM state. The blue and green spheres correspond to the majority and minority spin density, respectively.

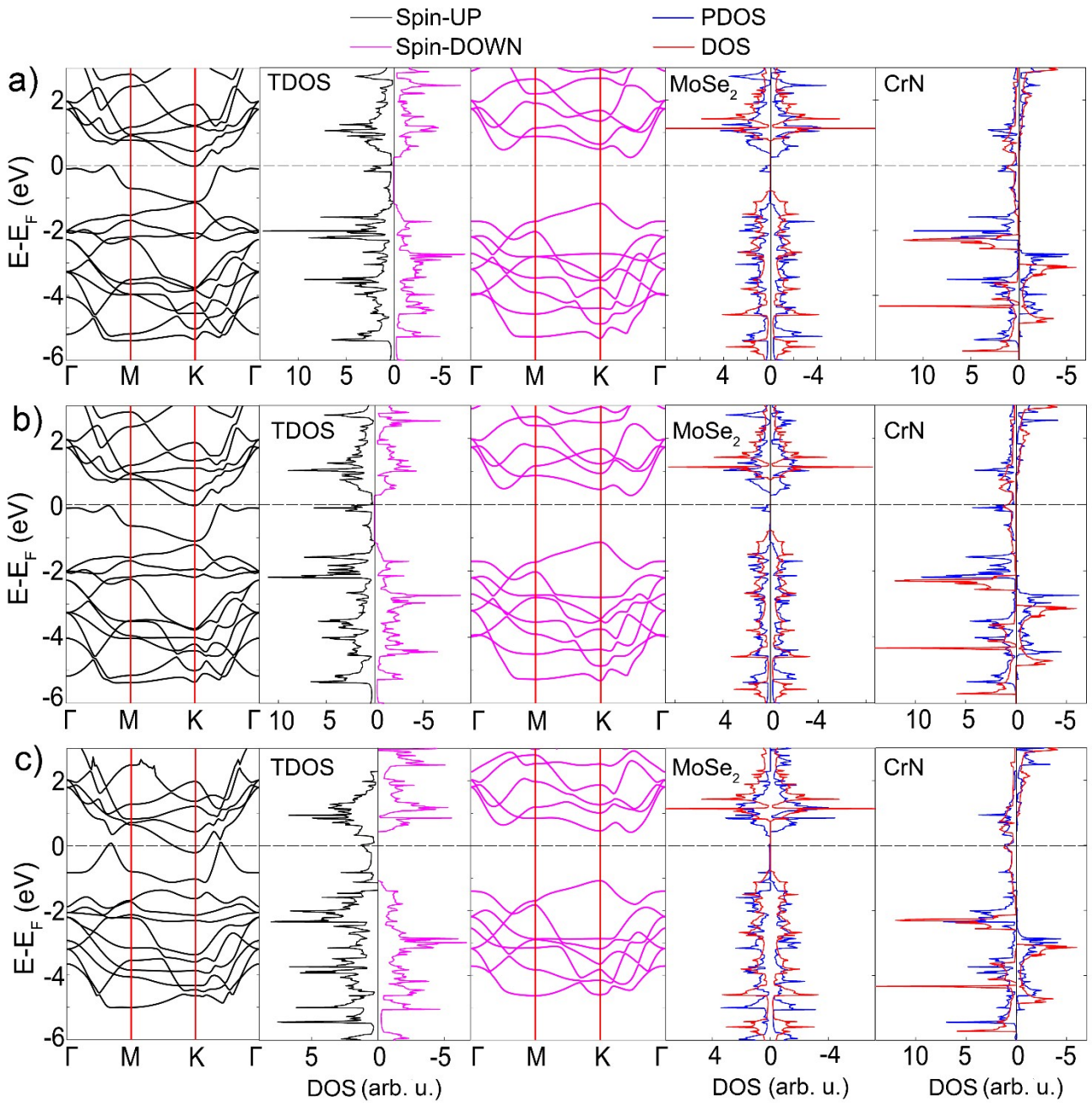

Figure S5. Band structures (spin-up and spin-down are black and pink) and densities of states. (a) Cr_[Se]–N_[Mo], (b) Cr_[Se]–N_[hex] and (c) Cr_[hex]–N_[Mo] configurations. DOSes of freestanding $MoSe_2$ and *h*-CrN are presented in red and PDOSes of $MoSe_2$ and *h*-CrN sheets are presented in blue.

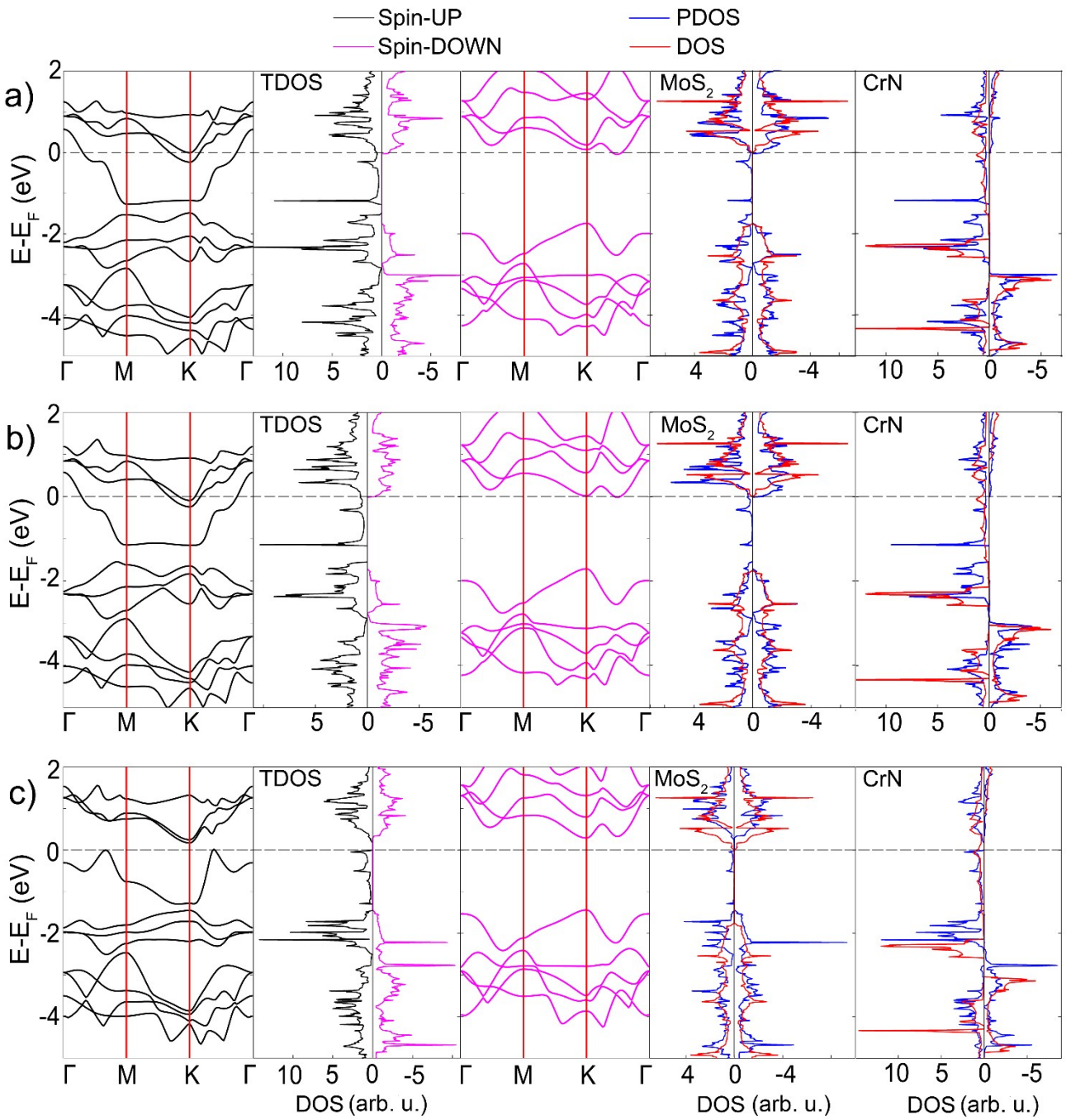

Figure S6. Band structures (spin-up and spin-down are black and pink) and densities of states. (a) Cr_[S]–N_[Mo], (b) Cr_[S]–N_[hex] and (c) Cr_[hex]–N_[Mo] configurations. DOSes of freestanding $MoSe_2$ and *h*-CrN are presented in red and PDOSes of MoS_2 and *h*-CrN sheets are presented in blue.

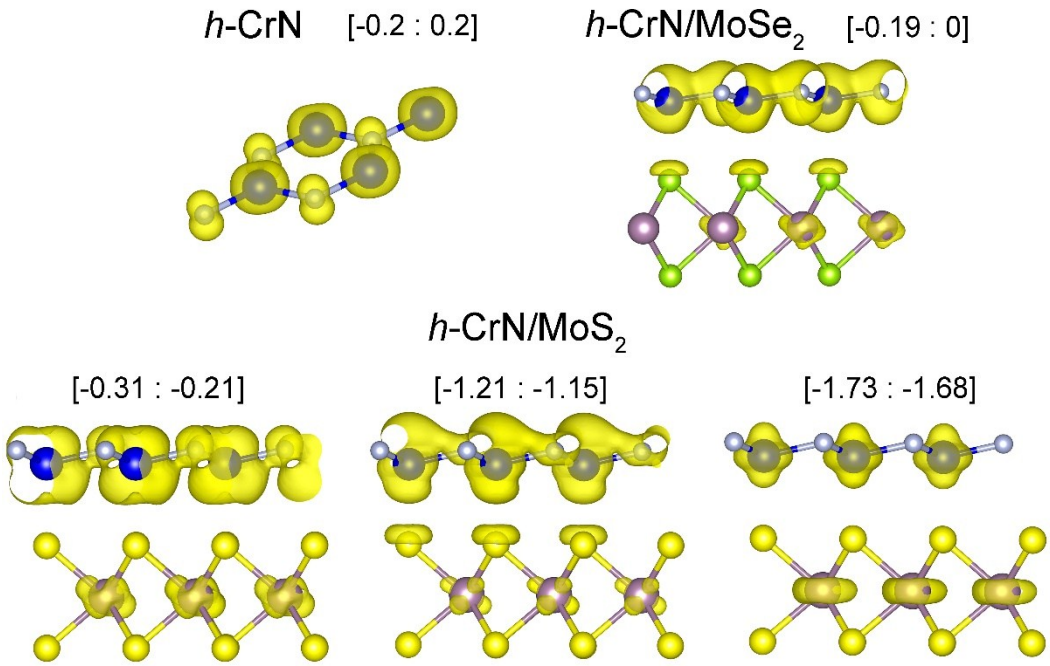

Figure S7. Spatial charge distribution of *h*-CrN, *h*-CrN/$MoSe_2$, *h*-CrN/MoS_2 in appropriative energy regions.

References

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