Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Electronic and Structural Properties of Adsorbed Non-Metallic Atoms on Magnesium Chloride Monolayers

Igo T. Lima,[1] *Ricardo Gargano*,[2] *Silvete Guerini*,[3] and *Edson N. C. Paura.*[4,*]

[1] Federal University of Maranhão, 65080-805, São Luis, MA, Brazil.

[2] Institute of Physics, University of Brasilia, Campus Darcy Ribeiro, Brasilia, Brazil.

[3] Department of Physics, Federal University of Maranhão, 65080-805, São Luis, MA, Brazil.

[4] Federal University of Maranhão, 65800-000, Balsas, MA, Brazil.

List of Figures & Tables

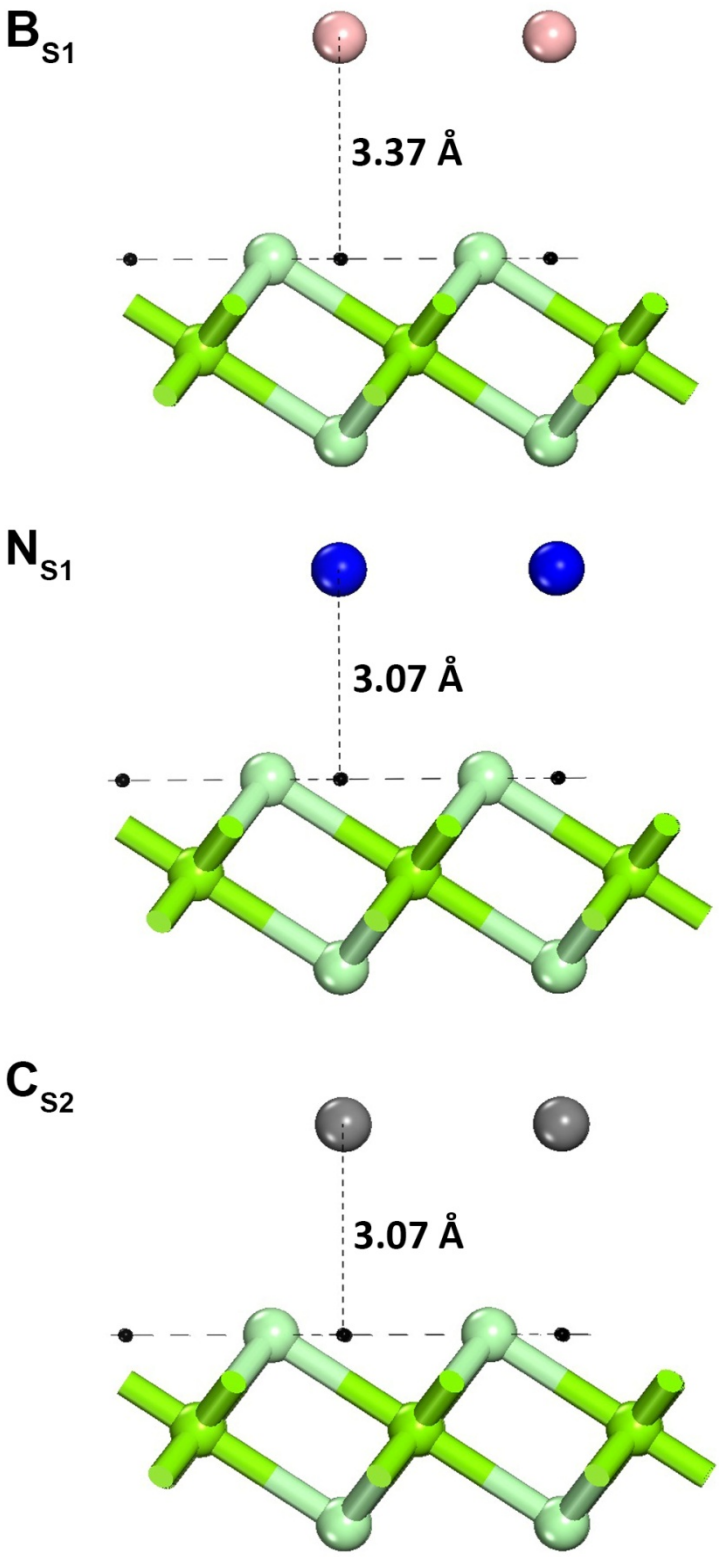

Figure S1. Optimized atomic structures of the planes formed by doped $MgCl_2$ monolayer with boron atoms (B_{S1} configuration), with nitrogen atoms (N_{S1} conguration), and carbon atoms (C_{S2} conguration).

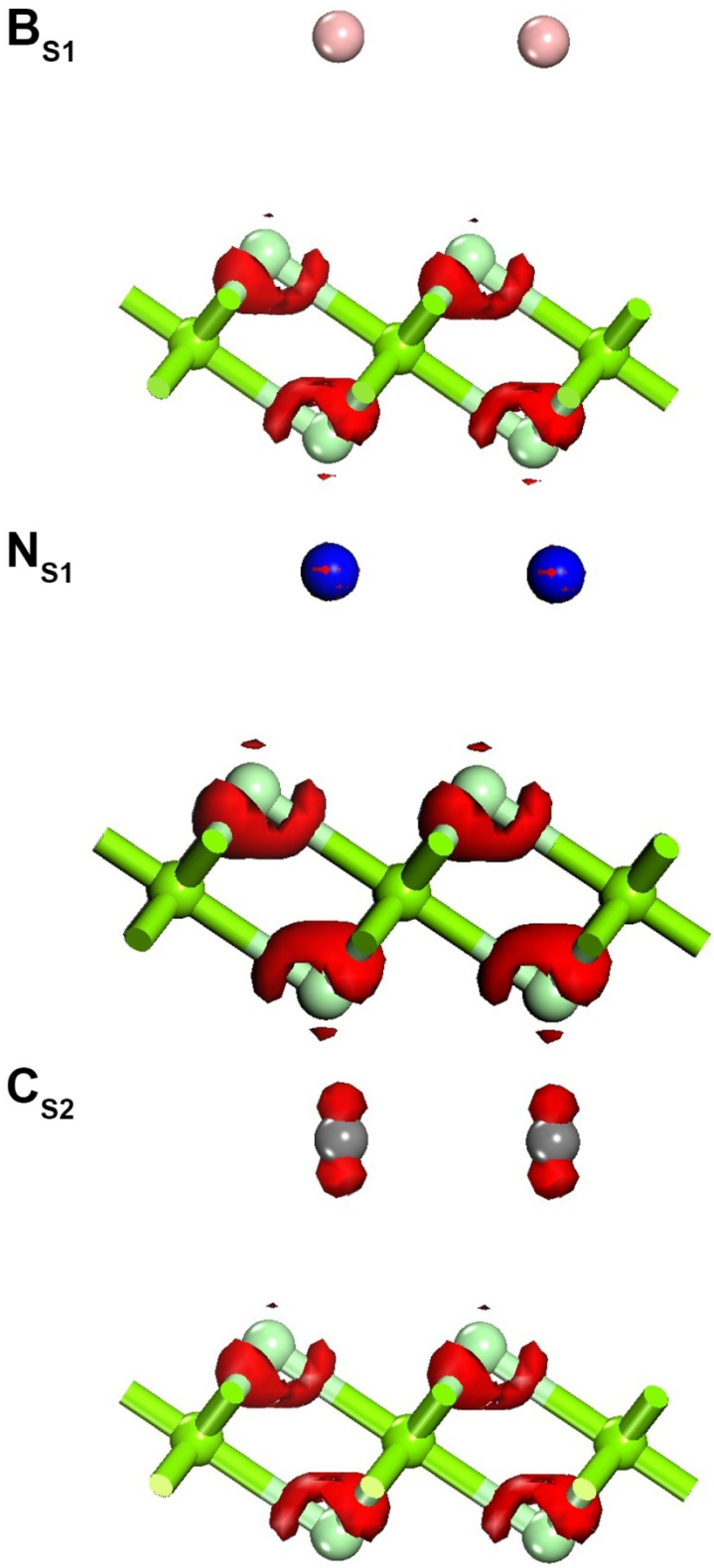

Figure S2. Density of deformed charge of the $MgCl_2$ monolayers doped with boron atoms (B_{S1} configuration), with nitrogen atoms (N_{S1} configuration), and carbon atoms (C_{S2} configurations). The dark green, light green, pink, blue and gray spheres represent the Mo, Cl, B, N and C atoms, respectively.

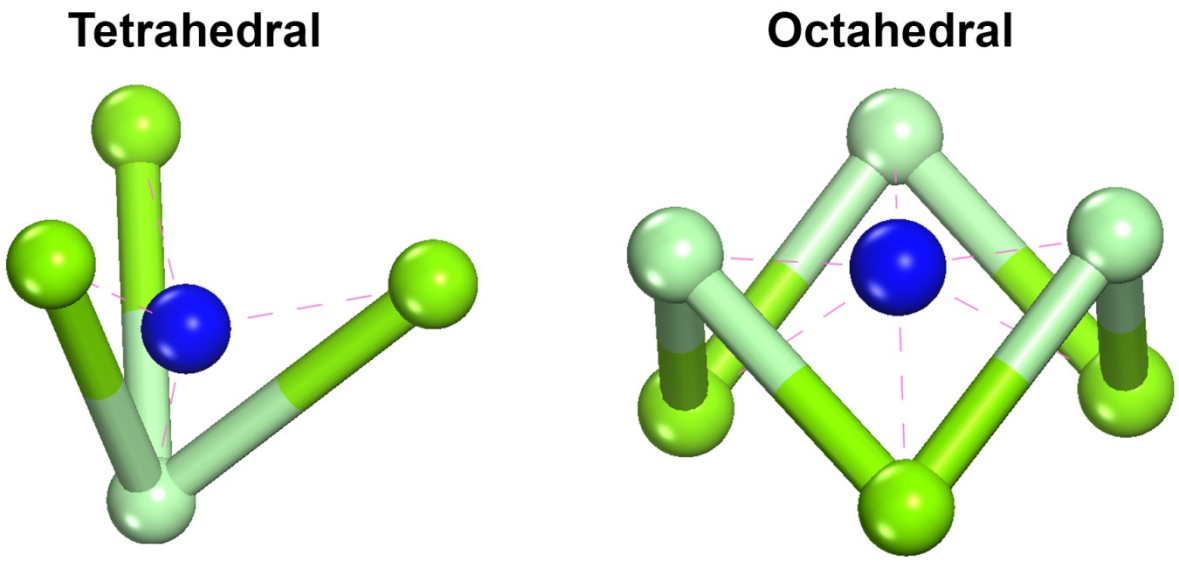

Figure S3. Extracted fragments from the doped monolayer with nitrogen atoms representing the tetrahedral configuration (left) and the octahedral configuration (right). The doped monolayer with carbon atoms presents similar configurations and the doped monolayer with boron atoms only presents octahedral configuration.

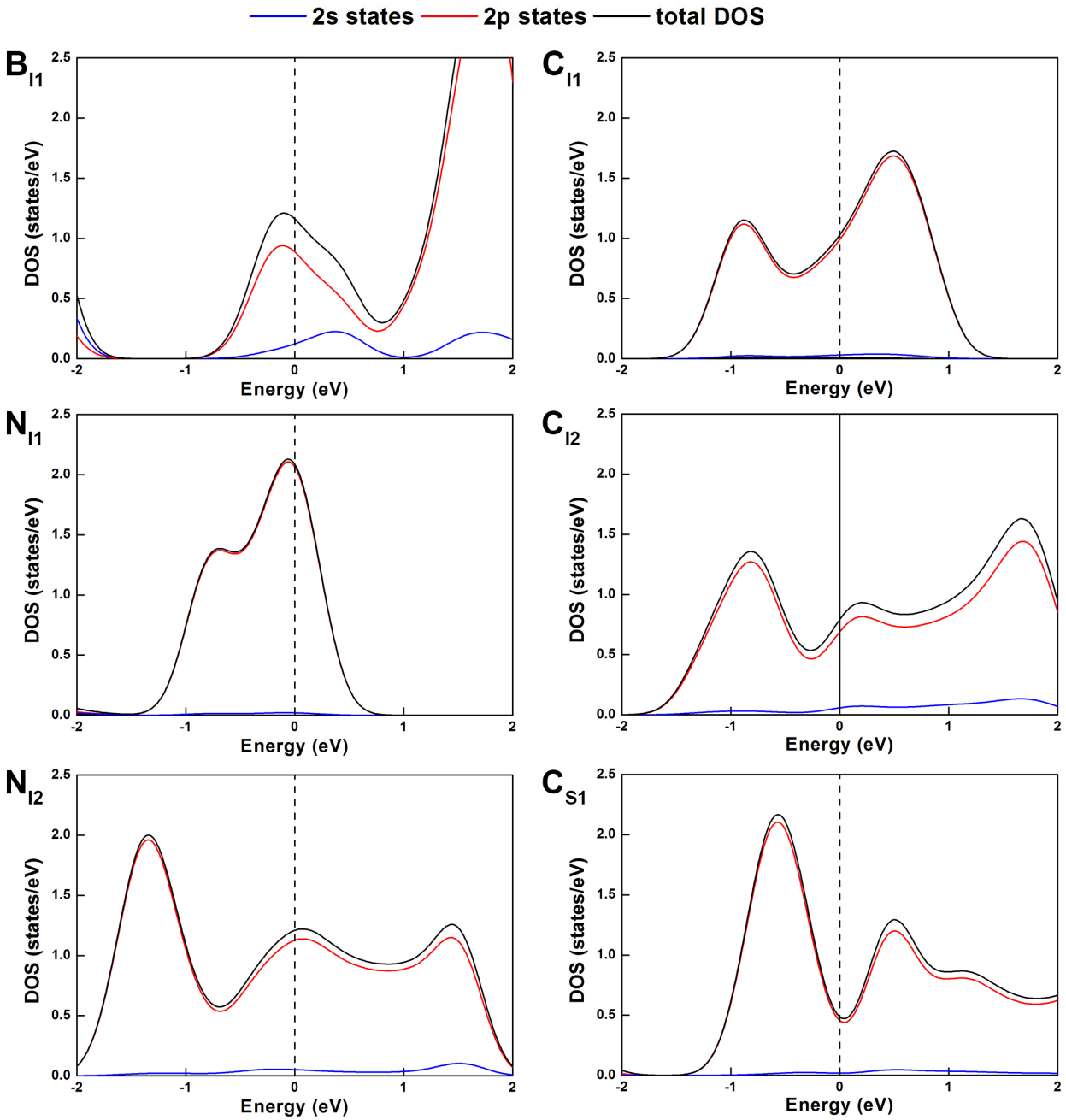

Figure S4: Total Density of States and Projected State Density only for of the dopant atoms present in the monolayer: boron atom (B_{I1}), nitrogen atoms (N_{I1} and N_{I2}) and carbon atoms (C_{I1}, C_{I2} and C_{S1}). The vertical dashed line represents the Fermi level.

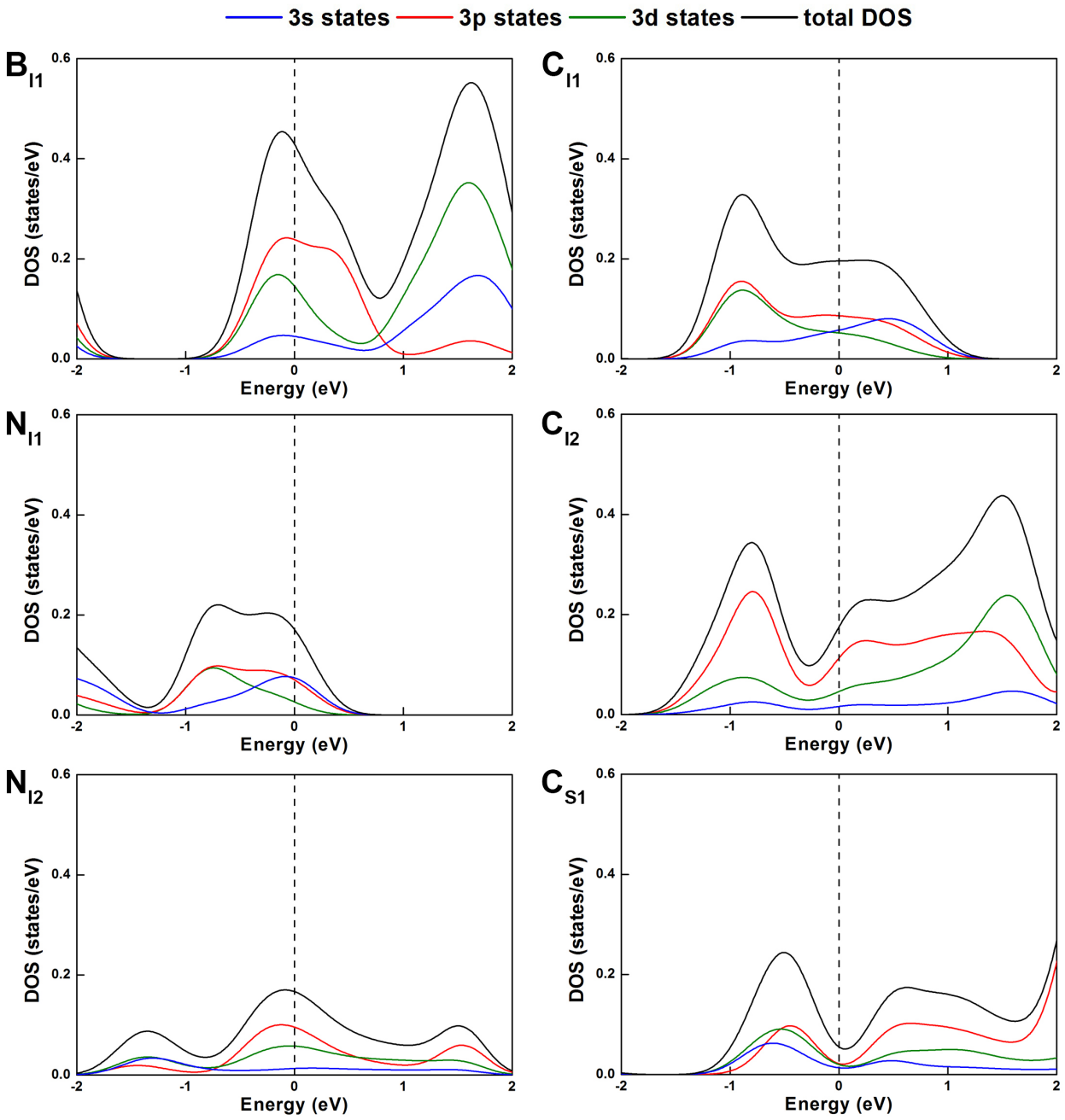

Figure S5: Total Density of States and Projected State Density only for the magnesium atoms present in the monolayer in the different configurations studied. The vertical dashed line represents the Fermi level.

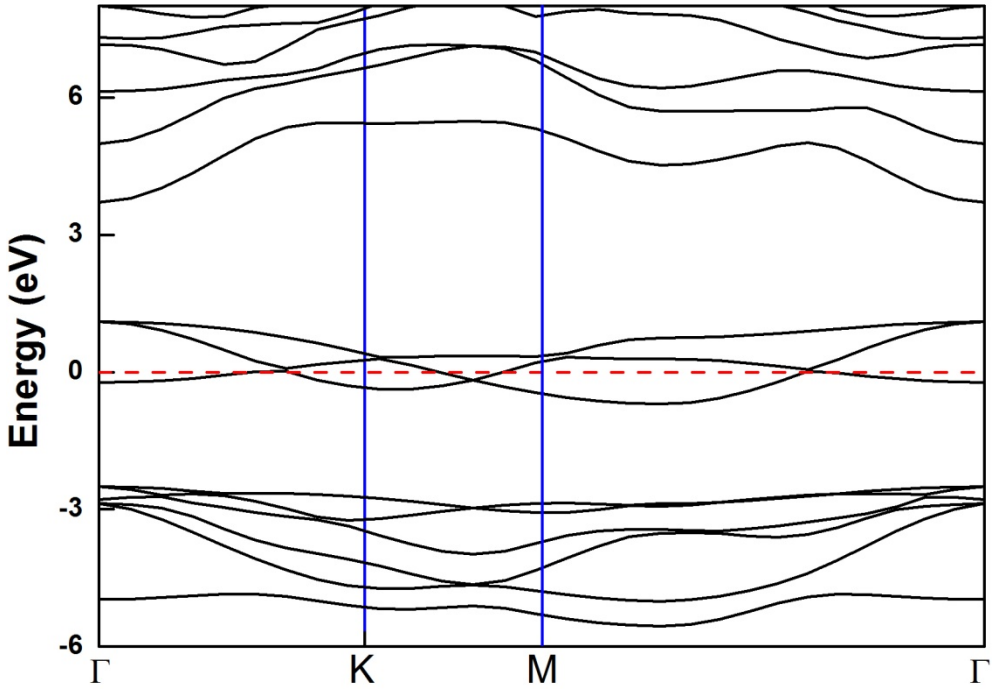

Figure S6. Structure of bands of $MgCl_2$ monolayer doped with nitrogen atoms in the B_{S1} configuration. The red dash line represents the Fermi level.

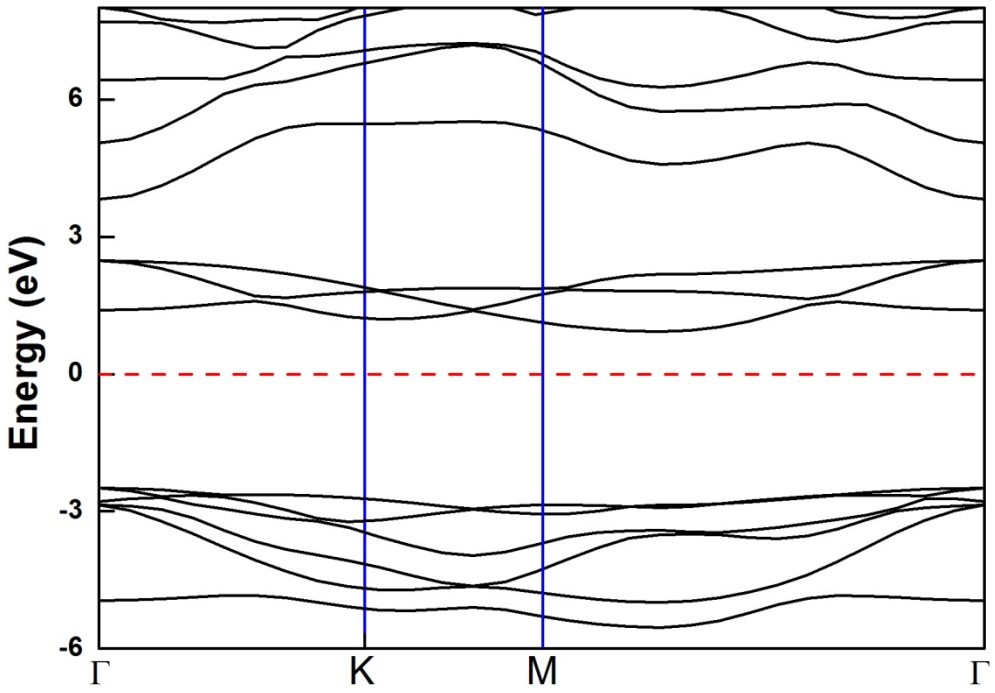

Figure S7. Structure of bands of $MgCl_2$ monolayer doped with nitrogen atoms in the N_{S1} configuration. The red dash line represents the Fermi level.

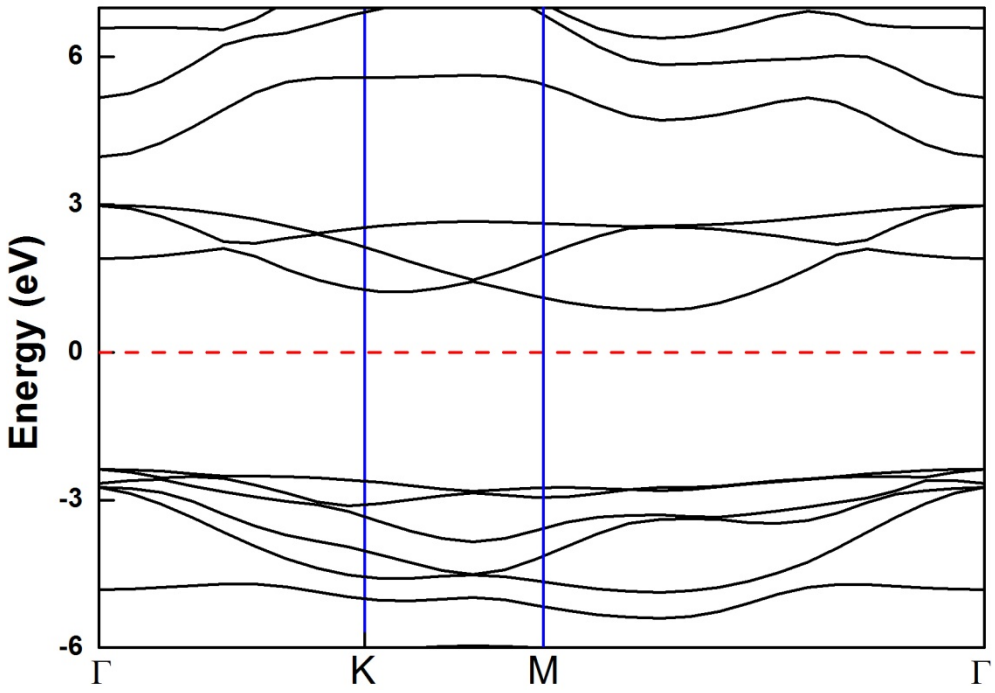

Figure S8. Structure of bands of $MgCl_2$ monolayer doped with carbon atoms in the C_{S2} configuration. The red dash line represents the Fermi level.

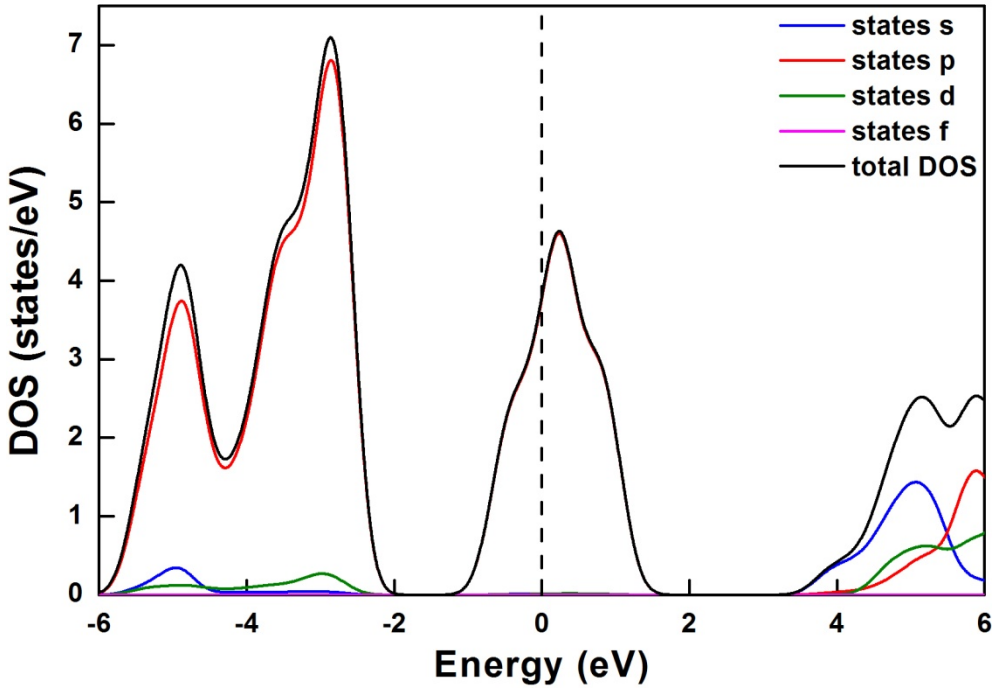

Figure S9. Total Density of States and Projected State Density of $MgCl_2$ monolayer doped with nitrogen atoms in the B_{S1} configuration. The vertical dashed line represents the Fermi level.

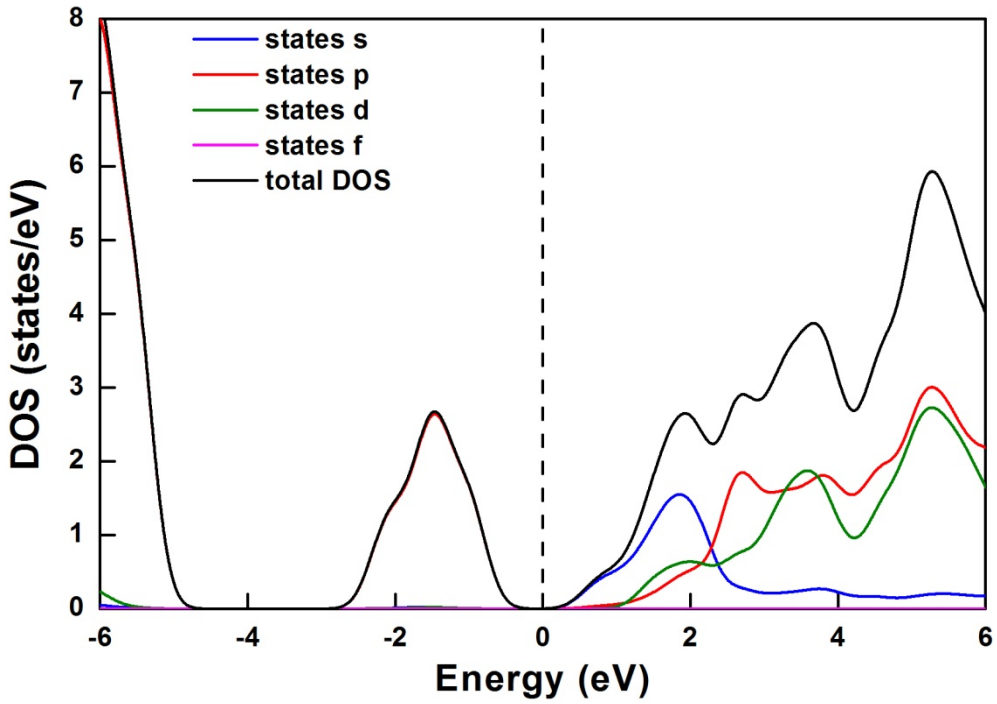

Figure S10. Total Density of States and Projected State Density of $MgCl_2$ monolayer doped with nitrogen atoms in the N_{S1} configuration. The vertical dashed line represents the Fermi level.

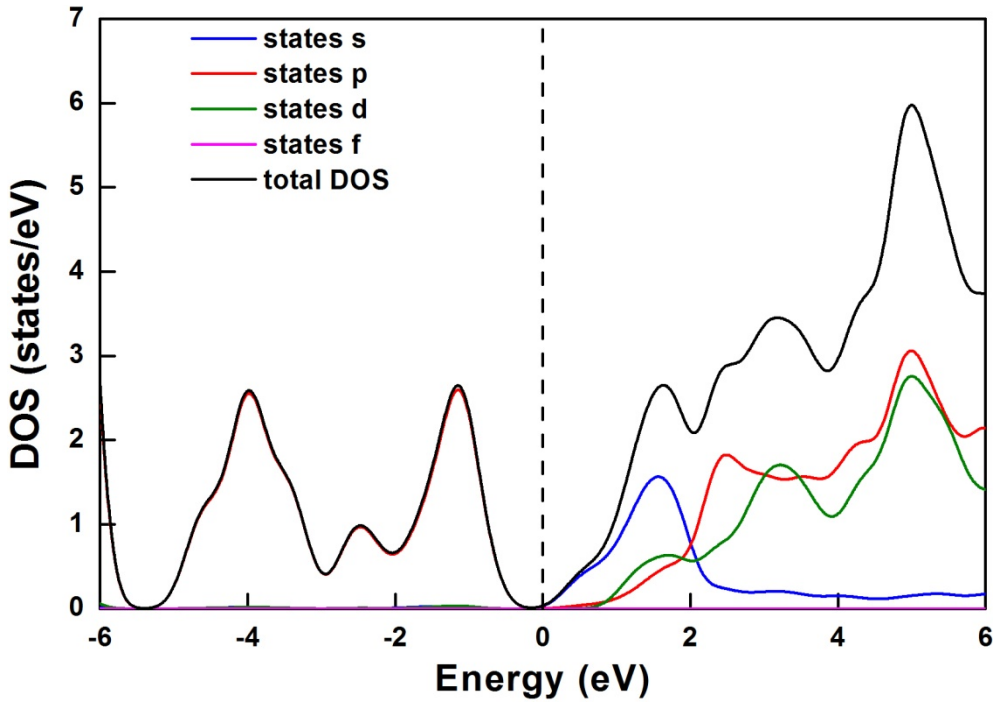

Figure S11. Total Density of States and Projected State Density of $MgCl_2$ monolayer doped with carbon atoms in the C_{S2} configuration. The vertical dashed line represents the Fermi level.