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Structural and Electronic Properties of $LaTiO_2N$ with O/N Disorder[1] WEI KANG, MARK S. HYBERTSEN, Center for Functional Nanomaterials, Brookhaven National Lab — $LaTiO_2N$ is an attractive candidate photocatalyst for water-splitting, showing strong absorption in the visible range with an optical gap about 2.1 eV and catalytic activity for hydrogen and oxygen evolution in the presence of auxiliary co-catalysts. It is also a good prototype suitable for theoretical study. It has a small unit cell while exhibiting several key characteristics found in the more complex oxides and oxynitrides synthesized in the search for improved photo-catalysts. This includes the reduced band gap and the disorder in one of the components, the O/N anion sublattice. We study the structural properties using a first-principles cluster expansion method. Our results reveal that at the temperatures characteristic of synthesis and annealing conditions, the occupation of O/N in $LaTiO_2N$ is intrinsically disordered. However the structure retains residual long-range order, in agreement with anion site occupancies measured in powder neutron diffraction. Short-range order in the O/N occupation is also observed. We use many-body perturbation theory to study the electronic and optical properties for some low-energy structures. The fundamental gap is found about 0.5 eV lower than the apparent absorption edge observed in experiments.

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