**First-principles theory of defect spins in w-AlN for quantum information and sensing technologies**[1] HOSUNG SEO, MARCO GOVONI, GIULIA GALLI, The Institute for Molecular Engineering, The University of Chicago — The detection and coherent manipulations of the single nitrogen-vacancy defect spin in diamond [1] attracted a tremendous amount of attention for possible applications in quantum computing and metrology. In addition, these results stimulated an active search for other materials, which may exhibit defect spins with similar properties. We present a systematic study aimed at searching for localized triplet spin states in $n-$type $w-$AlN. We use a combination of *ab-initio* calculations based on density functional and many-body perturbation theory and model calculations with an extended Hubbard Hamiltonian whose parameters were derived from first-principles. We consider five native defects: $V_N$, $V_{Al}$, $O_N$, $V_{Al}O_N$, and $V_{Al}V_N$. We investigated the defect charge and spin-state energetics and we discuss the effect of strain fields on the defect stability. We also discuss possible initialization schemes utilizing spin-dependent optical transitions and possible decoherence dynamics for qubits in $w-$AlN, which is most likely dominated by Al nuclear spin bath.

[1] A. Gruber et al., Science 276, 2012 (1997); F. Jelezko et al., Phys. Rev. Lett 93, 130501 (2004).

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